H-M Weng

List of Publications by Year in Descending Order

187 papers	19,082 citations	56 h-index	137 g-index
208 ext. papers	23,375 ext. citations	7.2 avg, IF	6.99 L-index

#	Paper	IF	Citations
187	Unconventional Materials: the mismatch between electronic charge centers and atomic positions. *Science Bulletin*, **2022**,	10.6	4
186	Flat-Band-Induced Anomalous Anisotropic Charge Transport and Orbital Magnetism in Kagome Metal CoSn.. *Physical Review Letters*, **2022**, 128, 096601	7.4	1
185	Extremely low-energy collective modes in a quasi-one-dimensional topological system. *Science China: Physics, Mechanics and Astronomy*, **2022**, 65, 1	3.6	
184	Unprotected quadratic band crossing points and quantum anomalous Hall effect in FeB2 monolayer. *Science China: Physics, Mechanics and Astronomy*, **2022**, 65, 1	3.6	0
183	RTGW2020: An efficient implementation of the multi-orbital Gutzwiller method with general local interactions. *Computer Physics Communications*, **2022**, 276, 108348	4.2	
182	Physical realization of topological Roman surface by spin-induced ferroelectric polarization in cubic lattice.. *Nature Communications*, **2022**, 13, 2373	17.4	1
181	High-harmonic generation in Weyl semimetal □WP crystals. *Nature Communications*, **2021**, 12, 6437	17.4	3
180	Topological insulators in the NaCaBi family with large spin-orbit coupling gaps. *Physical Review Research*, **2021**, 3,	3.9	1
179	High-throughput screening for Weyl semimetals with S4 symmetry. *Science Bulletin*, **2021**, 66, 667-675	10.6	6
178	Application of topological quantum chemistry in electrides. *Physical Review B*, **2021**, 103,	3.3	8
177	Unusual electronic structure of Dirac material BaMnSb2 revealed by angle-resolved photoemission spectroscopy*. *Chinese Physics B*, **2021**, 30, 067403	1.2	1
176	Electronic structure examination of the topological properties of CaMnSb2 by angle-resolved photoemission spectroscopy. *Physical Review B*, **2021**, 103,	3.3	1
175	Metallization of Quantum Material GaTaSe at High Pressure. *Journal of Physical Chemistry Letters*, **2021**, 12, 5601-5607	6.4	1
174	Facet Engineering to Regulate Surface States of Topological Crystalline Insulator Bismuth Rhombic Dodecahedrons for Highly Energy Efficient Electrochemical CO Reduction. *Advanced Materials*, **2021**, 33, e2008373	24	22
173	Electronic structures and topological properties in nickelates Ni O. *National Science Review*, **2021**, 8, nwaa288	23.178	21
172	Spin excitations and spin wave gap in the ferromagnetic Weyl semimetal Co3Sn2S2. *Science China: Physics, Mechanics and Astronomy*, **2021**, 64, 1	3.6	10
171	Observation and control of the weak topological insulator state in ZrTe. *Nature Communications*, **2021**, 12, 406	17.4	13

170	Hybrid nodal chain in an orthorhombic graphene network. *Physical Review B*, **2021**, 103,	3.3	3
169	Anisotropic magnetoelastic response in the magnetic Weyl semimetal Co3Sn2S2. *Science China: Physics, Mechanics and Astronomy*, **2021**, 64, 1	3.6	6
168	A combinatory ferroelectric compound bridging simple ABO and A-site-ordered quadruple perovskite. *Nature Communications*, **2021**, 12, 747	17.4	9
167	Spectroscopic evidence for the realization of a genuine topological nodal-line semimetal in LaSbTe. *Physical Review B*, **2021**, 103,	3.3	4
166	High-Throughput Screening of Element-Doped Carbon Nanotubes Toward an Optimal One-Dimensional Superconductor. *Journal of Physical Chemistry Letters*, **2021**, 12, 6667-6675	6.4	0
165	First Principle Calculation of the Effective Zeeman Couplings in Topological Materials **2021**, 263-281		1
164	Spin-polarized gap in the magnetic Weyl semimetal Co3Sn2S2. *Physical Review B*, **2021**, 104,	3.3	1
163	Giant nonlinear Hall effect in twisted bilayer WTe2. *Npj Quantum Materials*, **2021**, 6,	5	5
162	Pentagraphite C8 : An all- sp2 topological nodal-line semimetal. *Physical Review B*, **2021**, 104,	3.3	2
161	Superconductivity and Fermi-surface nesting in the candidate Dirac semimetal NbC. *Physical Review B*, **2020**, 102,	3.3	9
160	Quantum Oscillations and Electronic Structure in the Large-Chern-Number Topological Chiral Semimetal PtGa. *Chinese Physics Letters*, **2020**, 37, 107504	1.8	4
159	Topological semimetal in an sp2 sp3 hybridized carbon network with nodal rings. *Physical Review B* , **2020**, 101,	3.3	8
158	Layer construction of topological crystalline insulator LaSbTe. *Science China: Physics, Mechanics and Astronomy*, **2020**, 63, 1	3.6	4
157	Signature of Dirac semimetal states in gray arsenic studied by de Haas van Alphen and Shubnikov de Haas quantum oscillations. *Physical Review B*, **2020**, 101,	3.3	1
156	Sub-picosecond photo-induced displacive phase transition in two-dimensional MoTe2. *Npj 2D Materials and Applications*, **2020**, 4,	8.8	18
155	Non-Fermi-liquid behavior and saddlelike flat band in the layered ferromagnet AlFe2B2. *Physical Review B*, **2020**, 101,	3.3	2
154	Topological metals induced by the Zeeman effect. *Physical Review B*, **2020**, 101,	3.3	8
153	Inelastic Electron Tunneling in 2H-Ta_{x}Nb_{1-x}Se_{2} Evidenced by Scanning Tunneling Spectroscopy. *Physical Review Letters*, **2020**, 124, 106403	7.4	1

152	Magnetic Semimetals and Quantized Anomalous Hall Effect in EuB_{6}. *Physical Review Letters*, **2020**, 124, 076403	7.4	25
151	Magnetization-Induced Band Shift in Ferromagnetic Weyl Semimetal Co_{3}Sn_{2}S_{2}. *Physical Review Letters*, **2020**, 124, 077403	7.4	22
150	Emergence of Nontrivial Low-Energy Dirac Fermions in Antiferromagnetic EuCd As. *Advanced Materials*, **2020**, 32, e1907565	24	14
149	Chiral terahertz wave emission from the Weyl semimetal TaAs. *Nature Communications*, **2020**, 11, 720	17.4	47
148	Weyl semimetals with S4 symmetry. *Physical Review B*, **2020**, 101,	3.3	5
147	Crystal and electronic structure of GaTa4Se8 from first-principles calculations. *Physical Review B*, **2020**, 102,	3.3	3
146	Pressure effect on the anomalous Hall effect of ferromagnetic Weyl semimetal Co3Sn2S2. *Physical Review Materials*, **2020**, 4,	3.2	5
145	Magnetic and electronic properties of a topological nodal line semimetal candidate: HoSbTe. *Physical Review Materials*, **2020**, 4,	3.2	5
144	Diagnosis scheme for topological degeneracies crossing high-symmetry lines. *Physical Review Research*, **2020**, 2,	3.9	9
143	RSAVS superconductors: Materials with a superconducting state that is robust against large volume shrinkage. *Physical Review Materials*, **2020**, 4,	3.2	1
142	Insight of the Influence of Magnetic-Field Direction on Magneto-Plasmonic Interfaces for Tuning Photocatalytical Performance of Semiconductors. *Journal of Physical Chemistry Letters*, **2020**, 11, 9931-9937	6.4	7
141	Atomically Resolved Edge States on a Layered Ferroelectric Oxide. *ACS Applied Materials & Interfaces*, **2020**, 12, 4150-4154	9.5	6
140	Topological electronic structure in the antiferromagnet HoSbTe. *Physical Review B*, **2020**, 102,	3.3	6
139	Non-Abelian reciprocal braiding of Weyl points and its manifestation in ZrTe. *Nature Physics*, **2020**, 16, 1137-1143	16.2	20
138	Topological phase transition in the layered magnetic compound MnSb2Te4: Spin-orbit coupling and interlayer coupling dependence. *Physical Review B*, **2020**, 102,	3.3	25
137	Type-II Dirac Semimetal State in a Superconductor Tantalum Carbide. *Chinese Physics Letters*, **2020**, 37, 087103	1.8	3
136	BaHgSn: A Dirac semimetal with surface hourglass fermions. *Physical Review B*, **2020**, 101,	3.3	1
135	Multi-loop node line states in ternary MgSrSi-type crystals. *Npj Computational Materials*, **2019**, 5,	10.9	7

134	Two-dimensional spin□valley-coupled Dirac semimetals in functionalized SbAs monolayers. *Materials Horizons*, **2019**, 6, 781-787	14.4	21
133	Dirac nodal surfaces and nodal lines in ZrSiS. *Science Advances*, **2019**, 5, eaau6459	14.3	53
132	Lighting up Weyl semimetals. *Nature Materials*, **2019**, 18, 428-429	27	10
131	Three-Dimensional Crystalline Modification of Graphene in all-sp Hexagonal Lattices with or without Topological Nodal Lines. *Journal of Physical Chemistry Letters*, **2019**, 10, 2515-2521	6.4	11
130	Symmetry-enforced chiral hinge states and surface quantum anomalous Hall effect in the magnetic axion insulator Bi2□SmxSe3. *Nature Physics*, **2019**, 15, 577-581	16.2	59
129	Observation of unconventional chiral fermions with long Fermi arcs in CoSi. *Nature*, **2019**, 567, 496-499	50.4	129
128	Realization of low-energy type-II Dirac fermions in (Ir 1□x Pt x)Te 2 superconductors. *Chinese Physics B*, **2019**, 28, 037103	1.2	4
127	Topological nodal line semimetals in graphene network structures. *Advances in Physics: X*, **2019**, 4, 1625734	3.4	6
126	Experimental evidence of anomalously large superconducting gap on topological surface state of □Bi2Pd film. *Science Bulletin*, **2019**, 64, 1215-1221	10.6	12
125	Higher-Order Topology of the Axion Insulator EuIn_{2}As_{2}. *Physical Review Letters*, **2019**, 122, 256402	7.4	90
124	Topological nodal lines and hybrid Weyl nodes in YCoC2. *APL Materials*, **2019**, 7, 101109	5.7	8
123	Topological phases in pyrochlore thallium niobate Tl2Nb2O6+x. *Npj Computational Materials*, **2019**, 5,	10.9	6
122	Topological crystalline insulators with C2 rotation anomaly. *Physical Review Research*, **2019**, 1,	3.9	6
121	Catalogue of topological electronic materials. *Nature*, **2019**, 566, 475-479	50.4	354
120	Superconductivity in Topological Semimetal □TaN at High Pressure*. *Chinese Physics Letters*, **2019**, 36, 087401	1.8	7
119	Dirac Surface States in Intrinsic Magnetic Topological Insulators EuSn2As2 and MnBi2nTe3n+1. *Physical Review X*, **2019**, 9,	9.1	99
118	Chiral fermion reversal in chiral crystals. *Nature Communications*, **2019**, 10, 5505	17.4	17
117	Superconductivity induced at a point contact on the topological semimetal tungsten carbide. *Physical Review B*, **2019**, 100,	3.3	10

116	Quantum oscillations and electronic structure in the large Chern number semimetal RhSn. *Physical Review B*, **2019**, 100,	3.3	5
115	Quasiparticle interference evidence of the topological Fermi arc states in chiral fermionic semimetal CoSi. *Science Advances*, **2019**, 5, eaaw9485	14.3	15
114	Topological electronic states in HfRuP family superconductors. *Npj Computational Materials*, **2019**, 5,	10.9	7
113	Phononic Helical Nodal Lines with PT Protection in MoB_{2}. *Physical Review Letters*, **2019**, 123, 245302	7.4	20
112	Topological nodal-line semimetals in ferromagnetic rare-earth-metal monohalides. *Physical Review B*, **2019**, 99,	3.3	30
111	Orthorhombic carbon oC24: A novel topological nodal line semimetal. *Carbon*, **2018**, 133, 39-43	10.4	35
110	Topological Nodal-Net Semimetal in a Graphene Network Structure. *Physical Review Letters*, **2018**, 120, 026402	7.4	68
109	Three-component fermions with surface Fermi arcs in tungsten carbide. *Nature Physics*, **2018**, 14, 349-354	16.2	75
108	Double-Weyl Phonons in Transition-Metal Monosilicides. *Physical Review Letters*, **2018**, 120, 016401	7.4	124
107	Recent Progress in the Study of Topological Semimetals. *Journal of the Physical Society of Japan*, **2018**, 87, 041001	1.5	69
106	Topological Nodal States in Circuit Lattice. *Research*, **2018**, 2018, 6793752	7.8	56
105	Predicting Dirac semimetals based on sodium ternary compounds. *Npj Computational Materials*, **2018**, 4,	10.9	9
104	Topological phase transitions driven by strain in monolayer tellurium. *Physical Review B*, **2018**, 98,	3.3	22
103	Large intrinsic anomalous Hall effect in half-metallic ferromagnet CoSnS with magnetic Weyl fermions. *Nature Communications*, **2018**, 9, 3681	17.4	240
102	A Wide-Range Photosensitive Weyl Semimetal Single Crystal-TaAs. *Advanced Materials*, **2018**, 30, e1801372	24	24
101	Pressure-induced topological phase transitions and strongly anisotropic magnetoresistance in bulk black phosphorus. *Physical Review B*, **2017**, 95,	3.3	24
100	Topological nodal line semimetals in the CaP3 family of materials. *Physical Review B*, **2017**, 95,	3.3	142
99	Topologically Entangled Rashba-Split Shockley States on the Surface of Grey Arsenic. *Physical Review Letters*, **2017**, 118, 046802	7.4	20

98	Heavy Weyl Fermion State in CeRu4Sn6. *Physical Review X*, **2017**, 7,	9.1	30
97	Experimental evidence of hourglass fermion in the candidate nonsymmorphic topological insulator KHgSb. *Science Advances*, **2017**, 3, e1602415	14.3	78
96	Observation of three-component fermions in the topological semimetal molybdenum phosphide. *Nature*, **2017**, 546, 627-631	50.4	231
95	Electronic evidence of temperature-induced Lifshitz transition and topological nature in ZrTe. *Nature Communications*, **2017**, 8, 15512	17.4	131
94	Anomalous Magneto-Transport Behavior in Transition Metal Pentatelluride HfTe 5. *Chinese Physics Letters*, **2017**, 34, 037102	1.8	13
93	Noncollinear Magnetic Structure and Multipolar Order in Eu_{2}Ir_{2}O_{7}. *Physical Review Letters*, **2017**, 119, 187203	7.4	9
92	From Nodal Chain Semimetal to Weyl Semimetal in HfC. *Physical Review Letters*, **2017**, 119, 036401	7.4	99
91	Electronic structure of SrSnAs near the topological critical point. *Scientific Reports*, **2017**, 7, 6133	4.9	13
90	Robustness of topological states with respect to lattice instability in the nonsymmorphic topological insulator KHgSb. *Physical Review B*, **2017**, 96,	3.3	1
89	Theoretical prediction of two-dimensional functionalized MXene nitrides as topological insulators. *Physical Review B*, **2017**, 96,	3.3	50
88	Interaction-driven quantum anomalous Hall effect in halogenated hematite nanosheets. *Physical Review B*, **2017**, 96,	3.3	10
87	d Orbital Topological Insulator and Semimetal in the Antifluorite CuS Family: Contrasting Spin Helicities, Nodal Box, and Hybrid Surface States. *Journal of Physical Chemistry Letters*, **2017**, 8, 3506-3511	6.4	48
86	Conetronics in 2D metal-organic frameworks: double/half Dirac cones and quantum anomalous Hall effect. *2D Materials*, **2017**, 4, 015015	5.9	31
85	Topological nodal line semimetals predicted from first-principles calculations. *Frontiers of Physics*, **2017**, 12, 1	3.7	91
84	A new member of the topological semimetals family. *National Science Review*, **2017**, 4, 798-799	10.8	5
83	Observation of Weyl nodes and Fermi arcs in tantalum phosphide. *Nature Communications*, **2016**, 7, 11006	17.4	224
82	Compensated Semimetal LaSb with Unsaturated Magnetoresistance. *Physical Review Letters*, **2016**, 117, 127204	7.4	104
81	Electronic structure, Dirac points and Fermi arc surface states in three-dimensional Dirac semimetal Na 3 Bi from angle-resolved photoemission spectroscopy. *Chinese Physics B*, **2016**, 25, 077101	1.2	14

80	Node-surface and node-line fermions from nonsymmorphic lattice symmetries. *Physical Review B*, **2016**, 93,	3.3	167
79	Determining the chirality of Weyl fermions from circular dichroism spectra in time-dependent angle-resolved photoemission. *Physical Review B*, **2016**, 93,	3.3	19
78	Topological semimetals with triply degenerate nodal points in β-phase tantalum nitride. *Physical Review B*, **2016**, 93,	3.3	187
77	Body-Centered Orthorhombic C_{16}: A Novel Topological Node-Line Semimetal. *Physical Review Letters*, **2016**, 116, 195501	7.4	129
76	Predicted Quantum Topological Hall Effect and Noncoplanar Antiferromagnetism in K_{0.5}RhO_{2}. *Physical Review Letters*, **2016**, 116, 256601	7.4	44
75	Evidence for Topological Edge States in a Large Energy Gap near the Step Edges on the Surface of ZrTe5. *Physical Review X*, **2016**, 6,	9.1	82
74	Emergence of topological bands on the surface of ZrSnTe crystal. *Physical Review B*, **2016**, 93,	3.3	50
73	Topological nodal line semimetals. *Chinese Physics B*, **2016**, 25, 117106	1.2	358
72	Topological node-line semimetal in compressed black phosphorus. *Physical Review B*, **2016**, 94,	3.3	89
71	Topological semimetals predicted from first-principles calculations. *Journal of Physics Condensed Matter*, **2016**, 28, 303001	1.8	202
70	Spontaneous Formation of a Superconductor-Topological Insulator-Normal Metal Layered Heterostructure. *Advanced Materials*, **2016**, 28, 5013-7	24	22
69	Giant semiclassical magnetoresistance in high mobility TaAs2 semimetal. *Applied Physics Letters*, **2016**, 108, 042105	3.4	56
68	Observation of Fermi arc and its connection with bulk states in the candidate type-II Weyl semimetal WTe2. *Physical Review B*, **2016**, 94,	3.3	158
67	Coexistence of Weyl fermion and massless triply degenerate nodal points. *Physical Review B*, **2016**, 94,	3.3	140
66	Pseudospin, real spin, and spin polarization of photoemitted electrons. *Physical Review B*, **2016**, 94,	3.3	5
65	Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides. *Physical Review X*, **2015**, 5,	9.1	968
64	Model Hamiltonian for topological Kondo insulator SmB6. *New Journal of Physics*, **2015**, 17, 023012	2.9	19
63	Electronic structure of transition metal dichalcogenides PdTe 2 and Cu 0.05 PdTe 2 superconductors obtained by angle-resolved photoemission spectroscopy. *Chinese Physics B*, **2015**, 24, 067401	1.2	16

62	Quantum spin Hall effect in two-dimensional transition-metal dichalcogenide haeckelites. *Physical Review B*, **2015**, 91,	3.3	75
61	Identification of Topological Surface State in PdTe 2 Superconductor by Angle-Resolved Photoemission Spectroscopy. *Chinese Physics Letters*, **2015**, 32, 067303	1.8	47
60	Quantum anomalous Hall effect and related topological electronic states. *Advances in Physics*, **2015** , 64, 227-282	18.4	251
59	Observation of Weyl nodes in TaAs. *Nature Physics*, **2015**, 11, 724-727	16.2	683
58	Topological node-line semimetal in three-dimensional graphene networks. *Physical Review B*, **2015**, 92,	3.3	488
57	Large-gap two-dimensional topological insulator in oxygen functionalized MXene. *Physical Review B* , **2015**, 92,	3.3	169
56	Topological nature of the FeSe0.5Te0.5 superconductor. *Physical Review B*, **2015**, 92,	3.3	129
55	Two-dimensional oxide topological insulator with iron-pnictide superconductor LiFeAs structure. *Physical Review B*, **2015**, 92,	3.3	120
54	Topological Node-Line Semimetal and Dirac Semimetal State in Antiperovskite Cu3PdN. *Physical Review Letters*, **2015**, 115, 036807	7.4	524
53	Observation of Fermi-Arc Spin Texture in TaAs. *Physical Review Letters*, **2015**, 115, 217601	7.4	89
52	Observation of the Chiral-Anomaly-Induced Negative Magnetoresistance in 3D Weyl Semimetal TaAs. *Physical Review X*, **2015**, 5,	9.1	752
51	Evidence for Half-Metallicity in n-type HgCr2Se4. *Physical Review Letters*, **2015**, 115, 087002	7.4	52
50	Experimental Discovery of Weyl Semimetal TaAs. *Physical Review X*, **2015**, 5,	9.1	1167
49	Anomalous High-Energy Waterfall-Like Electronic Structure in 5 d Transition Metal Oxide Sr2IrO4 with a Strong Spin-Orbit Coupling. *Scientific Reports*, **2015**, 5, 13036	4.9	15
48	First-Principles Study on Cubic Pyrochlore Iridates Y2Ir2O7 and Pr2Ir2O7. *Journal of the Physical Society of Japan*, **2015**, 84, 073703	1.5	19
47	Large linear magnetoresistance in Dirac semimetal Cd3As2 with Fermi surfaces close to the Dirac points. *Physical Review B*, **2015**, 92,	3.3	139
46	A stable three-dimensional topological Dirac semimetal Cd3As2. *Nature Materials*, **2014**, 13, 677-81	27	1010
45	Topological crystalline Kondo insulator in mixed valence ytterbium borides. *Physical Review Letters*, **2014**, 112, 016403	7.4	123

44	Discovery of a three-dimensional topological Dirac semimetal, Na3Bi. *Science*, **2014**, 343, 864-7	33.3	1516
43	Exploration and prediction of topological electronic materials based on first-principles calculations. *MRS Bulletin*, **2014**, 39, 849-858	3.2	65
42	Transition-Metal Pentatelluride ZrTe5 and HfTe5: A Paradigm for Large-Gap Quantum Spin Hall Insulators. *Physical Review X*, **2014**, 4,	9.1	196
41	Direct observation of the spin texture in SmB6 as evidence of the topological Kondo insulator. *Nature Communications*, **2014**, 5, 4566	17.4	155
40	Optical spectroscopy study of Nd(O,F)BiS2 single crystals. *Physical Review B*, **2014**, 90,	3.3	16
39	Topological insulator to Dirac semimetal transition driven by sign change of spin-orbit coupling in thallium nitride. *Physical Review B*, **2014**, 90,	3.3	35
38	The electronic structure of NaIrO 3 , Mott insulator or band insulator?. *Europhysics Letters*, **2013**, 101, 27003	1.6	20
37	Three-dimensional Dirac semimetal and quantum transport in Cd3As2. *Physical Review B*, **2013**, 88,	3.3	1094
36	Correlated topological insulators with mixed valence. *Physical Review Letters*, **2013**, 110, 096401	7.4	245
35	Superconductivity in topological insulator Sb2Te3 induced by pressure. *Scientific Reports*, **2013**, 3, 2016	4.9	113
34	Introduction to Topological Insulators **2012**, 01, 31-36		2
33	Dirac semimetal and topological phase transitions in A3Bi (A=Na, K, Rb). *Physical Review B*, **2012**, 85,	3.3	1244
32	Superconductivity of topological matters induced via pressure. *Frontiers of Physics*, **2012**, 7, 193-199	3.7	27
31	Effect of Cleaving Temperature on the Surface and Bulk Fermi Surface of Sr 2 RuO 4 Investigated by High Resolution Angle-Resolved Photoemission. *Chinese Physics Letters*, **2012**, 29, 067401	1.8	3
30	Fermi surface sheet-dependent band splitting in Sr2RuO4 revealed by high-resolution angle-resolved photoemission spectroscopy. *Physical Review B*, **2012**, 86,	3.3	8
29	Magnetic ordering and multiferroicity in MnI2. *Physical Review B*, **2012**, 86,	3.3	19
28	Robustness of topological order and formation of quantum well states in topological insulators exposed to ambient environment. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 3694-8	11.5	139
27	Electronic structure of the delafossite-type CuMO2 (M = Sc, Cr, Mn, Fe, and Co): Optical absorption measurements and first-principles calculations. *Physical Review B*, **2011**, 84,	3.3	52

26	Chern semimetal and the quantized anomalous Hall effect in HgCr2Se4. *Physical Review Letters*, **2011**, 107, 186806	7.4	960
25	Pressure-induced superconductivity in topological parent compound Bi2Te3. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 24-8	11.5	236
24	Half-metallic surface states and topological superconductivity in NaCoO2 from first principles. *Physical Review B*, **2011**, 84,	3.3	27
23	Topological aspect and quantum magnetoresistance of Ag2Te. *Physical Review Letters*, **2011**, 106, 156808	7.4	155
22	Phase diagram of LaVO3 under epitaxial strain: Implications for thin films grown on SrTiO3 and LaAlO3 substrates. *Physical Review B*, **2010**, 82,	3.3	17
21	Dual spin filter effect in a zigzag graphene nanoribbon. *Physical Review B*, **2010**, 81,	3.3	109
20	Robust Dirac point in honeycomb-structure nanoribbons with zigzag edges. *Physical Review B*, **2010** , 81,	3.3	12
19	First-principles study of the rectifying properties of Pt/TiO2 interface. *Physical Review B*, **2009**, 80,	3.3	47
18	Revisiting magnetic coupling in transition-metal-benzene complexes with maximally localized Wannier functions. *Physical Review B*, **2009**, 79,	3.3	54
17	Evolution of magnetic circular dichroism of pure ZnTe in magnetic field: Spectral similarity between undoped and Cr-doped ZnTe. *Physical Review B*, **2008**, 77,	3.3	3
16	Tailoring Magnetic Properties in Transition Metal–Benzene Sandwich Clusters: Ways to Design Molecular Magnets. *Journal of the Physical Society of Japan*, **2008**, 77, 064301	1.5	10
15	Theoretical Analysis of Magnetic Coupling in Sandwich Clusters Vn(C6H6)n+1. *Journal of the Physical Society of Japan*, **2008**, 77, 014301	1.5	31
14	Spin-orbit interaction in Au structures of various dimensionalities. *Applied Physics Letters*, **2008**, 92, 023115	3.4	10
13	Ferromagnetism in HfO2 induced by hole doping: First-principles calculations. *Physical Review B*, **2006**, 73,	3.3	32
12	Nonlinear optical susceptibility of deformed achiral carbon nanotubes studied from first-principles calculations. *Applied Physics Letters*, **2006**, 89, 013102	3.4	6
11	Electronic structure and optical properties of layered perovskites Sr2MO4 (M=Ti, V, Cr, and Mn): An ab initio study. *Physical Review B*, **2006**, 74,	3.3	30
10	First principles investigation of the magnetic circular dichroism spectra of Co-doped anatase and rutile TiO2. *Physical Review B*, **2006**, 73,	3.3	40
9	Magneto-optical Kerr effects of half-metallic ferromagnetic transition metal chalcogenides in zinc-blende and wurtzite structures. *Physical Review B*, **2006**, 74,	3.3	14

8	Magnetic circular dichroism spectra in a II-VI diluted magnetic semiconductor Zn1−xCrxTe: First-principles calculations. *Physical Review B*, **2006**, 74,	3.3	8
7	First-principles investigation of transition-metal-doped group-IV semiconductors: RxY1−x (R=Cr,Mn,Fe;Y=Si,Ge). *Physical Review B*, **2005**, 71,	3.3	52
6	Electronic structure and symmetry of small clusters C28. *Computational and Theoretical Chemistry*, **2004**, 671, 93-95		3
5	Electronic structure and optical properties of the Co-doped anatase TiO2 studied from first principles. *Physical Review B*, **2004**, 69,	3.3	154
4	Optical properties of 4 Å single-walled carbon nanotubes inside the zeolite channels studied from first principles calculations. *European Physical Journal B*, **2003**, 32, 345-350	1.2	19
3	Electronic structure and linear optical properties of Sr(mathsf{_{2}})CuO(mathsf{_{2}})Cl(mathsf{_{2}}) studied from the first principles calculation. *European Physical Journal B*, **2003**, 35, 217-221	1.2	3
2	Band structure of MgB2 with different lattice constants. *Physical Review B*, **2001**, 65,	3.3	47
1	Progress, Advantages, and Challenges of Topological Material Catalysts. *Small Science*,2100106		4