Yugui Yao

List of Publications by Citations

202 papers	15,746 citations	54 h-index	123 g-index
221 ext. papers	18,802 ext. citations	6.5 avg, IF	6.89 L-index

#	Paper	IF	Citations
202	Quantum spin Hall effect in silicene and two-dimensional germanium. *Physical Review Letters*, **2011**, 107, 076802	7.4	1666
201	Evidence of silicene in honeycomb structures of silicon on Ag(111). *Nano Letters*, **2012**, 12, 3507-11	11.5	1055
200	Low-energy effective Hamiltonian involving spin-orbit coupling in silicene and two-dimensional germanium and tin. *Physical Review B*, **2011**, 84,	3.3	938
199	Epitaxial growth of single-domain graphene on hexagonal boron nitride. *Nature Materials*, **2013**, 12, 792-7	27	745
198	Spin-orbit gap of graphene: First-principles calculations. *Physical Review B*, **2007**, 75,	3.3	720
197	Evidence for Dirac fermions in a honeycomb lattice based on silicon. *Physical Review Letters*, **2012**, 109, 056804	7.4	577
196	Rise of silicene: A competitive 2D material. *Progress in Materials Science*, **2016**, 83, 24-151	42.2	548
195	First principles calculation of anomalous Hall conductivity in ferromagnetic bcc Fe. *Physical Review Letters*, **2004**, 92, 037204	7.4	545
194	Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides. *Physical Review B*, **2013**, 88,	3.3	526
193	Quantum anomalous Hall effect in graphene from Rashba and exchange effects. *Physical Review B*, **2010**, 82,	3.3	461
192	Electronic structures and theoretical modelling of two-dimensional group-VIB transition metal dichalcogenides. *Chemical Society Reviews*, **2015**, 44, 2643-63	58.5	398
191	Borophene as an extremely high capacity electrode material for Li-ion and Na-ion batteries. *Nanoscale*, **2016**, 8, 15340-7	7.7	272
190	Berry-phase effect in anomalous thermoelectric transport. *Physical Review Letters*, **2006**, 97, 026603	7.4	272
189	Valley-polarized quantum anomalous Hall effect in silicene. *Physical Review Letters*, **2014**, 112, 106802	7.4	248
188	Quantum spin Hall insulators and quantum valley Hall insulators of BiX/SbX (X=H, F, Cl and Br) monolayers with a record bulk band gap. *NPG Asia Materials*, **2014**, 6, e147-e147	10.3	216
187	Investigations on V2C and V2CX2 (X = F, OH) Monolayer as a Promising Anode Material for Li Ion Batteries from First-Principles Calculations. *Journal of Physical Chemistry C*, **2014**, 118, 24274-24281	3.8	215
186	Symmetry breaking of graphene monolayers by molecular decoration. *Physical Review Letters*, **2009**, 102, 135501	7.4	213

185	Engineering quantum anomalous/valley Hall states in graphene via metal-atom adsorption: An ab-initio study. *Physical Review B*, **2011**, 84,	3.3	188
184	Quantum anomalous Hall effect in single-layer and bilayer graphene. *Physical Review B*, **2011**, 83,	3.3	174
183	Intrinsic spin Hall effect in monolayers of group-VI dichalcogenides: A first-principles study. *Physical Review B*, **2012**, 86,	3.3	165
182	Topological aspect and quantum magnetoresistance of β-Ag2Te. *Physical Review Letters*, **2011**, 106, 156808	7.4	155
181	Theoretical prediction of MoN2 monolayer as a high capacity electrode material for metal ion batteries. *Journal of Materials Chemistry A*, **2016**, 4, 15224-15231	13	154
180	Predicted Unusual Magnetoresponse in Type-II Weyl Semimetals. *Physical Review Letters*, **2016**, 117, 077202	7.4	152
179	Half-Heusler topological insulators: A first-principles study with the Tran-Blaha modified Becke-Johnson density functional. *Physical Review B*, **2010**, 82,	3.3	141
178	Experimental realization of two-dimensional Dirac nodal line fermions in monolayer CuSi. *Nature Communications*, **2017**, 8, 1007	17.4	138
177	Linear magnetization dependence of the intrinsic anomalous Hall effect. *Physical Review Letters*, **2006**, 96, 037204	7.4	136
176	Two-dimensional topological insulator state and topological phase transition in bilayer graphene. *Physical Review Letters*, **2011**, 107, 256801	7.4	132
175	2D Electrides as Promising Anode Materials for Na-Ion Batteries from First-Principles Study. *ACS Applied Materials & Interfaces*, **2015**, 7, 24016-22	9.5	126
174	Large-gap quantum spin Hall insulator in single layer bismuth monobromide Bi4Br4. *Nano Letters*, **2014**, 14, 4767-71	11.5	125
173	Tailoring magnetic doping in the topological insulator Bi2Se3. *Physical Review Letters*, **2012**, 109, 266405	7.4	124
172	Microscopic theory of quantum anomalous Hall effect in graphene. *Physical Review B*, **2012**, 85,	3.3	115
171	Type-II nodal loops: Theory and material realization. *Physical Review B*, **2017**, 96,	3.3	110
170	Effects of strain on electronic and optic properties of holey two-dimensional C2N crystals. *Applied Physics Letters*, **2015**, 107, 231904	3.4	109
169	Low-energy effective Hamiltonian for giant-gap quantum spin Hall insulators in honeycomb X-hydride/halide (X=N-Bi) monolayers. *Physical Review B*, **2014**, 90,	3.3	102
168	Stability, electronic, and magnetic properties of the magnetically doped topological insulators Bi2Se3, Bi2Te3, and Sb2Te3. *Physical Review B*, **2013**, 88,	3.3	100

167	Ab initio calculation of the intrinsic spin Hall effect in semiconductors. *Physical Review Letters*, **2005**, 94, 226601	7.4	99
166	Interplay between different magnetisms in Cr-doped topological insulators. *ACS Nano*, **2013**, 7, 9205-12	16.7	94
165	Observation of Dirac cone warping and chirality effects in silicene. *ACS Nano*, **2013**, 7, 9049-54	16.7	83
164	Computational characterization of monolayer C3N: A two-dimensional nitrogen-graphene crystal. *Journal of Materials Research*, **2017**, 32, 2993-3001	2.5	82
163	Artificial gravity field, astrophysical analogues, and topological phase transitions in strained topological semimetals. *Npj Quantum Materials*, **2017**, 2,	5	80
162	Coherent wave-packet evolution in coupled bands. *Physical Review B*, **2005**, 72,	3.3	73
161	Promising ferroelectricity in 2D group IV tellurides: a first-principles study. *Applied Physics Letters*, **2017**, 111, 132904	3.4	72
160	Nonsymmorphic-symmetry-protected hourglass Dirac loop, nodal line, and Dirac point in bulk and monolayer X3SiTe6 (X = Ta, Nb). *Physical Review B*, **2018**, 97,	3.3	71
159	First-principles demonstration of superconductivity at 280 K in hydrogen sulfide with low phosphorus substitution. *Physical Review B*, **2016**, 93,	3.3	65
158	Even-odd layer-dependent magnetotransport of high-mobility Q-valley electrons in transition metal disulfides. *Nature Communications*, **2016**, 7, 12955	17.4	64
157	Formation of quantum spin Hall state on Si surface and energy gap scaling with strength of spin orbit coupling. *Scientific Reports*, **2014**, 4, 7102	4.9	62
156	Robust quantum anomalous Hall effect in graphene-based van der Waals heterostructures. *Physical Review B*, **2015**, 92,	3.3	61
155	Large magneto-optical Kerr effect in noncollinear antiferromagnets Mn3X(X=Rh,Ir,Pt). *Physical Review B*, **2015**, 92,	3.3	60
154	Quantum spin Hall and Z2 metallic states in an organic material. *Physical Review B*, **2014**, 90,	3.3	59
153	Twist angle-dependent conductivities across MoS/graphene heterojunctions. *Nature Communications*, **2018**, 9, 4068	17.4	59
152	Ultralow-temperature photochemical synthesis of atomically dispersed Pt catalysts for the hydrogen evolution reaction. *Chemical Science*, **2019**, 10, 2830-2836	9.4	58
151	Weak Topological Insulators and Composite Weyl Semimetals: Bi4X4 (X=Br, I). *Physical Review Letters*, **2016**, 116, 066801	7.4	56
150	Valley-dependent properties of monolayer MoSi2N4, WSi2N4, and MoSi2As4. *Physical Review B*, **2020**, 102,	3.3	55

149	Electronic, Dielectric, and Plasmonic Properties of Two-Dimensional Electride Materials X2N (X=Ca, Sr): A First-Principles Study. *Scientific Reports*, **2015**, 5, 12285	4.9	54
148	Robust ferroelectricity in two-dimensional SbN and BiP. *Nanoscale*, **2018**, 10, 7984-7990	7.7	52
147	Tunable ferroelectricity and anisotropic electric transport in monolayer □GeSe. *Physical Review B*, **2018**, 97,	3.3	49
146	Effect of doping and strain modulations on electron transport in monolayer MoS2. *Physical Review B*, **2014**, 90,	3.3	49
145	From Type-II Triply Degenerate Nodal Points and Three-Band Nodal Rings to Type-II Dirac Points in Centrosymmetric Zirconium Oxide. *Journal of Physical Chemistry Letters*, **2017**, 8, 5792-5797	6.4	49
144	Intervalley coupling by quantum dot confinement potentials in monolayer transition metal dichalcogenides. *New Journal of Physics*, **2014**, 16, 105011	2.9	49
143	Ferromagnetic hybrid nodal loop and switchable type-I and type-II Weyl fermions in two dimensions. *Physical Review B*, **2020**, 102,	3.3	49
142	Fano-Enhanced Circular Dichroism in Deformable Stereo Metasurfaces. *Advanced Materials*, **2020**, 32, e1907077	24	47
141	Peierls-Nabarro model of interfacial misfit dislocation: An analytic solution. *Physical Review B*, **1999**, 59, 8232-8236	3.3	47
140	Probing the topological phase transition via density oscillations in silicene and germanene. *Physical Review B*, **2014**, 89,	3.3	46
139	Phonon-mediated superconductivity in silicene predicted by first-principles density functional calculations. *Europhysics Letters*, **2013**, 104, 36001	1.6	45
138	Two-dimensional spin-orbit Dirac point in monolayer HfGeTe. *Physical Review Materials*, **2017**, 1,	3.2	45
137	Engineering symmetry breaking in 2D layered materials. *Nature Reviews Physics*, **2021**, 3, 193-206	23.6	45
136	Monolayer group-III monochalcogenides by oxygen functionalization: a promising class of two-dimensional topological insulators. *Npj Quantum Materials*, **2018**, 3,	5	43
135	Spin-polarized and valley helical edge modes in graphene nanoribbons. *Physical Review B*, **2011**, 84,	3.3	43
134	Quantum Anomalous Hall Effect in Graphene-based Heterostructure. *Scientific Reports*, **2015**, 5, 10629	4.9	41
133	Strain tuning of topological band order in cubic semiconductors. *Physical Review B*, **2012**, 85,	3.3	41
132	First-principles calculation of topological invariants within the FP-LAPW formalism. *Computer Physics Communications*, **2012**, 183, 1849-1859	4.2	41

131	Tunable hyperbolic dispersion and negative refraction in natural electride materials. *Physical Review B*, **2017**, 95,	3.3	40
130	Discovery of Weyl Nodal Lines in a Single-Layer Ferromagnet. *Physical Review Letters*, **2019**, 123, 116401	7.4	37
129	Possible electric-field-induced superconducting states in doped silicene. *Scientific Reports*, **2015**, 5, 8203	4.9	37
128	Multilayered Electride CaN Electrode via Compression Molding Fabrication for Sodium Ion Batteries. *ACS Applied Materials & Interfaces*, **2017**, 9, 6666-6669	9.5	36
127	Valley-polarized quantum anomalous Hall phases and tunable topological phase transitions in half-hydrogenated Bi honeycomb monolayers. *Physical Review B*, **2015**, 91,	3.3	36
126	Tunable magneto-optical effects in hole-doped group-IIIA metal-monochalcogenide monolayers. *2D Materials*, **2017**, 4, 015017	5.9	35
125	Topological phases in gated bilayer graphene: Effects of Rashba spin-orbit coupling and exchange field. *Physical Review B*, **2013**, 87,	3.3	33
124	Tunable half-metallic magnetism in an atom-thin holey two-dimensional C2N monolayer. *Journal of Materials Chemistry C*, **2017**, 5, 8424-8430	7.1	33
123	Electronic structures of graphene layers on a metal foil: The effect of atomic-scale defects. *Applied Physics Letters*, **2013**, 103, 143120	3.4	31
122	Robust edge photocurrent response on layered type II Weyl semimetal WTe. *Nature Communications*, **2019**, 10, 5736	17.4	30
121	Valley-polarized quantum anomalous Hall phase and disorder-induced valley-filtered chiral edge channels. *Physical Review B*, **2015**, 91,	3.3	29
120	Engineering topological surface states and giant Rashba spin splitting in BiTeI/Bi2Te3 heterostructures. *Scientific Reports*, **2014**, 4, 3841	4.9	28
119	Graphene Foam: Uniaxial Tension Behavior and Fracture Mode Based on a Mesoscopic Model. *ACS Nano*, **2017**, 11, 8988-8997	16.7	28
118	Three-dimensional topological insulators: A review on host materials. *Science China: Physics, Mechanics and Astronomy*, **2012**, 55, 2199-2212	3.6	26
117	Spin-order dependent anomalous Hall effect and magneto-optical effect in the noncollinear antiferromagnets Mn3XN with X=Ga, Zn, Ag, or Ni. *Physical Review B*, **2019**, 99,	3.3	25
116	Electric field controlled spin- and valley-polarized edge states in silicene with extrinsic Rashba effect. *Physical Review B*, **2015**, 92,	3.3	25
115	Theoretical evidence of the Berry-phase mechanism in anomalous Hall transport: First-principles studies of CuCr2Se4□Brx. *Physical Review B*, **2007**, 75,	3.3	25
114	Topological edge states in single- and multi-layer Bi4Br4. *New Journal of Physics*, **2015**, 17, 015004	2.9	24

113	Chen et al. reply. *Physical Review Letters*, **2013**, 110, 229702	7.4	24
112	Topological magnetic phase in LaMnO3 (111) bilayer. *Physical Review B*, **2015**, 92,	3.3	24
111	Quantum anomalous Hall effect in stanene on a nonmagnetic substrate. *Physical Review B*, **2016**, 94,	3.3	24
110	Origin of charge density wave in the kagome metal CsV3Sb5 as revealed by optical spectroscopy. *Physical Review B*, **2021**, 104,	3.3	24
109	Two-dimensional spin□valley-coupled Dirac semimetals in functionalized SbAs monolayers. *Materials Horizons*, **2019**, 6, 781-787	14.4	21
108	Nodal Line Spin-Gapless Semimetals and High-Quality Candidate Materials. *Physical Review Letters*, **2020**, 124, 016402	7.4	21
107	High throughput screening for two-dimensional topological insulators. *2D Materials*, **2018**, 5, 045023	5.9	21
106	Topological, Valleytronic, and Optical Properties of Monolayer PbS. *Advanced Materials*, **2017**, 29, 1604788	24	20
105	Fully Spin-Polarized Nodal Loop Semimetals in Alkaline Metal Monochalcogenide Monolayers. *Journal of Physical Chemistry Letters*, **2019**, 10, 3101-3108	6.4	20
104	Hole-doped room-temperature superconductivity in H3S1-xZ (Z=C, Si). *Materials Today Physics*, **2020**, 15, 100330	8	20
103	Almost ideal nodal-loop semimetal in monoclinic CuTeO3 material. *Physical Review B*, **2018**, 97,	3.3	20
102	Topological Nodal Line Electrides: Realization of an Ideal Nodal Line State Nearly Immune from Spin□rbit Coupling. *Journal of Physical Chemistry C*, **2019**, 123, 25871-25876	3.8	19
101	Multiple energy scales and anisotropic energy gap in the charge-density-wave phase of the kagome superconductor CsV3Sb5. *Physical Review B*, **2021**, 104,	3.3	19
100	Electromechanically reconfigurable optical nano-kirigami. *Nature Communications*, **2021**, 12, 1299	17.4	19
99	High-Throughput Screening of Magnetic Antiperovskites. *Chemistry of Materials*, **2018**, 30, 6983-6991	9.6	19
98	Magnetotransport Properties of Graphene Nanoribbons with Zigzag Edges. *Physical Review Letters*, **2018**, 120, 216601	7.4	19
97	Temperature-driven evolution of critical points, interlayer coupling, and layer polarization in bilayer MoS2. *Physical Review B*, **2018**, 97,	3.3	18
96	Pressure-induced phase transitions and superconductivity in a quasi-1-dimensional topological crystalline insulator □BiBr. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 17696-17700	11.5	18

95	Memristive Crossbar Arrays for Storage and Computing Applications. *Advanced Intelligent Systems*, **2021**, 3, 2100017	6	18
94	Electronic nature of chiral charge order in the kagome superconductor CsV3Sb5. *Physical Review B*, **2021**, 104,	3.3	17
93	Self-assembled chiral phosphorus nanotubes from phosphorene: a molecular dynamics study. *RSC Advances*, **2017**, 7, 24647-24651	3.7	16
92	Topological magneto-optical effects and their quantization in noncoplanar antiferromagnets. *Nature Communications*, **2020**, 11, 118	17.4	16
91	Simulations of twisted bilayer orthorhombic black phosphorus. *Physical Review B*, **2017**, 96,	3.3	16
90	Large magneto-optical effects in hole-doped blue phosphorene and gray arsenene. *Nanoscale*, **2017**, 9, 17405-17414	7.7	16
89	Time-reversal-invariant topological superconductivity in n-doped BiH. *Physical Review B*, **2015**, 91,	3.3	16
88	Topological p+ip superconductivity in doped graphene-like single-sheet materials BC3. *Physical Review B*, **2015**, 92,	3.3	16
87	Relationships between strain and band structure in Si(001) and Si(110) nanomembranes. *Physical Review B*, **2009**, 80,	3.3	16
86	Theory of orbital magnetization in disordered systems. *Physical Review B*, **2012**, 86,	3.3	16
85	High-Throughput Screening and Automated Processing toward Novel Topological Insulators. *Journal of Physical Chemistry Letters*, **2018**, 9, 6224-6231	6.4	16
84	Weakened interlayer coupling in two-dimensional MoSe2 flakes with screw dislocations. *Nano Research*, **2019**, 12, 1900-1905	10	15
83	From node-line semimetals to large-gap quantum spin Hall states in a family of pentagonal group-IVA chalcogenide. *Physical Review B*, **2018**, 97,	3.3	15
82	Manipulation of the dielectric properties of diamond by an ultrashort laser pulse. *Physical Review B*, **2017**, 95,	3.3	15
81	Transport tuning of photonic topological edge states by optical cavities. *Physical Review A*, **2019**, 99,	2.6	14
80	Topological metallic phases in spin–orbit coupled bilayer systems. *New Journal of Physics*, **2014**, 16, 123015	2.9	14
79	Mirror protected multiple nodal line semimetals and material realization. *Physical Review B*, **2018**, 98,	3.3	13
78	First-principles investigations on the Berry phase effect in spin–orbit coupling materials. *Computational Materials Science*, **2016**, 112, 428-447	3.2	12

77	Ab initio pair potentials at metal-ceramic interfaces. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1999**, 256, 391-398	2.3	12
76	Direct identification of Mott Hubbard band pattern beyond charge density wave superlattice in monolayer 1T-NbSe. *Nature Communications*, **2021**, 12, 1978	17.4	12
75	Type-III Weyl semimetals: (TaSe4)2I. *Physical Review B*, **2021**, 103,	3.3	12
74	Observation of Topological Edge States at the Step Edges on the Surface of Type-II Weyl Semimetal TaIrTe. *ACS Nano*, **2019**, 13, 9571-9577	16.7	11
73	Twofold symmetry of c-axis resistivity in topological kagome superconductor CsVSb with in-plane rotating magnetic field. *Nature Communications*, **2021**, 12, 6727	17.4	11
72	Cat(s)-cradle-like Dirac semimetals in layer groups with multiple screw axes: Application to two-dimensional borophene and borophane. *Physical Review B*, **2018**, 98,	3.3	11
71	Composition and phase engineering of metal chalcogenides and phosphorous chalcogenides. *Nature Materials*,	27	11
70	Strongly distinct electrical response between circular and valley polarization in bilayer transition metal dichalcogenides. *Physical Review B*, **2019**, 99,	3.3	10
69	Decay characteristics of two-dimensional islands on strongly anisotropic surfaces. *Physical Review B* , **2002**, 66,	3.3	10
68	Quantum transport properties in single crystals of Bi4I4. *Physical Review Materials*, **2018**, 2,	3.2	10
67	Giant anomalous Nernst effect in noncollinear antiferromagnetic Mn-based antiperovskite nitrides. *Physical Review Materials*, **2020**, 4,	3.2	10
66	Experimental observation of node-line-like surface states in LaBi. *Physical Review B*, **2018**, 97,	3.3	9
65	Thickness-dependent magneto-optical effects in hole-doped GaS and GaSe multilayers: a first-principles study. *New Journal of Physics*, **2018**, 20, 043048	2.9	9
64	Pressure-tunable large anomalous Hall effect of the ferromagnetic kagome-lattice Weyl semimetal Co3Sn2S2. *Physical Review B*, **2019**, 100,	3.3	9
63	Robust Fano resonance in the photonic valley Hall states. *Physical Review A*, **2021**, 103,	2.6	9
62	SpaceGroupIrep: A package for irreducible representations of space group. *Computer Physics Communications*, **2021**, 265, 107993	4.2	9
61	Two-dimensional antiferromagnetic Dirac fermions in monolayer TaCoTe2. *Physical Review B*, **2019**, 100,	3.3	8
60	Controlling global stochasticity in the standard map. *Physical Review E*, **2000**, 61, 7219-22	2.4	8

59	Magnetization-direction tunable nodal-line and Weyl phases. *Physical Review B*, **2018**, 98,	3.3	8
58	Weyl Nodal Point-Line Fermion in Ferromagnetic EuBi. *Journal of Physical Chemistry Letters*, **2019**, 10, 2508-2514	6.4	7
57	Experimental evidence of monolayer AlB2 with symmetry-protected Dirac cones. *Physical Review B*, **2020**, 101,	3.3	7
56	Nodal-line semimetal states in the positive-electrode material of a lead-acid battery: Lead dioxide family and its derivatives. *Physical Review B*, **2018**, 98,	3.3	7
55	Robust circular polarization of indirect Q-K transitions in bilayer 3R WS2. *Physical Review B*, **2019**, 100,	3.3	7
54	Tunable Intrinsic Plasmons due to Band Inversion in Topological Materials. *Physical Review Letters*, **2017**, 119, 266804	7.4	7
53	Negative differential magnetization in ultrathin Fe on vicinal W(100). *Physical Review B*, **2003**, 67,	3.3	7
52	Signature of band inversion in the antiferromagnetic phase of axion insulator candidate EuIn2As2. *Physical Review Research*, **2020**, 2,	3.9	7
51	Double Dirac nodal line semimetal with a torus surface state. *Physical Review B*, **2021**, 103,	3.3	7
50	Sign-reversible valley-dependent Berry phase effects in 2D valley-half-semiconductors. *Npj Computational Materials*, **2021**, 7,	10.9	7
49	Density functional study of weak ferromagnetism in a thick BiCrO3 film. *Journal of Applied Physics*, **2011**, 109, 103905	2.5	6
48	THE MULTISCALE MODEL COMBINING ELASTIC THEORY WITH AB INITIO CALCULATIONS FOR METAL CERAMIC INTERFACES. *Modern Physics Letters B*, **2008**, 22, 3135-3143	1.6	6
47	Unconventional Pairing Induced Anomalous Transverse Shift in Andreev Reflection. *Physical Review Letters*, **2018**, 121, 176602	7.4	6
46	Tantalum disulfide quantum dots: preparation, structure, and properties. *Nanoscale Research Letters*, **2020**, 15, 20	5	5
45	Control of the hyperbolic dispersion of dielectrics by an ultrashort laser pulse. *Physical Review B*, **2018**, 97,	3.3	5
44	Controlling hamiltonian chaos by adaptive integrable mode coupling. *Physical Review E*, **2000**, 62, 2135-9	2.4	5
43	Artificial Propeller Chirality and Counterintuitive Reversal of Circular Dichroism in Twisted Meta-molecules. *Nano Letters*, **2021**, 21, 6828-6834	11.5	5
42	Double reflection and tunneling resonance in a topological insulator: Towards the quantification of warping strength by transport. *Physical Review B*, **2017**, 96,	3.3	4

41	Type-II topological metals. *Frontiers of Physics*, **2020**, 15, 1	3.7	4
40	The Kapitza Resistance Across Grain Boundary by Molecular Dynamics Simulation. *Nanoscale and Microscale Thermophysical Engineering*, **2006**, 10, 387-398	3.7	4
39	Topologically nontrivial interband plasmons in type-II Weyl semimetal MoTe2. *New Journal of Physics*, **2020**, 22, 103032	2.9	4
38	Transport signatures of temperature-induced chemical potential shift and Lifshitz transition in layered type-II Weyl semimetal TaIrTe4. *2D Materials*, **2021**, 8, 015020	5.9	4
37	Strong magneto-optical effect and anomalous transport in the two-dimensional van der Waals magnets FenGeTe2 (n=3, 4, 5). *Physical Review B*, **2021**, 104,	3.3	4
36	MagneticTB: A package for tight-binding model of magnetic and non-magnetic materials. *Computer Physics Communications*, **2022**, 270, 108153	4.2	4
35	Physical Fingerprints of the 2O-t□ Phase in Phosphorene Stacking. *Journal of Physical Chemistry Letters*, **2019**, 10, 3190-3196	6.4	3
34	A tunable and unidirectional one-dimensional electronic system Nb2n+1SinTe4n+2. *Npj Quantum Materials*, **2020**, 5,	5	3
33	Observation of One-Dimensional Dirac Fermions in Silicon Nanoribbons.. *Nano Letters*, **2022**, 22, 695-701	11.5	3
32	Weyl Monoloop Semi-Half-Metal and Tunable Anomalous Hall Effect. *Nano Letters*, **2021**, 21, 8749-8755	11.5	3
31	Van der Waals Epitaxial Growth of Two-Dimensional BiOBr Flakes with Dendritic Structures for the Hydrogen Evolution Reaction. *ACS Applied Energy Materials*, **2020**, 3, 11848-11854	6.1	3
30	Weyl nodal-line surface half-metal in CaFeO3. *Physical Review B*, **2021**, 103,	3.3	3
29	Ultralong Single-Crystal □Bi4Br4 Nanobelts with a High Current-Carrying Capacity by Mechanical Exfoliation. *Journal of Physical Chemistry C*,	3.8	3
28	Tunable magneto-optical effect, anomalous Hall effect, and anomalous Nernst effect in the two-dimensional room-temperature ferromagnet 1T□CrTe2. *Physical Review B*, **2021**, 103,	3.3	3
27	Trigonal warping induced unusual spin texture and strong spin polarization in graphene with the Rashba effect. *Physical Review B*, **2018**, 97,	3.3	2
26	An efficient method for hybrid density functional calculation with spin□orbit coupling. *Computer Physics Communications*, **2018**, 224, 90-97	4.2	2
25	Liu et al. reply. *Physical Review Letters*, **2015**, 114, 099702	7.4	2
24	Strain effect on the instability of island formation in submonolayer heteroepitaxy. *Europhysics Letters*, **2009**, 86, 16001	1.6	2

23	Determination of detonation characteristics by laser-induced plasma spectra and micro-explosion dynamics.. *Optics Express*, **2022**, 30, 4718-4736	3.3	2
22	Systematic investigation of emergent particles in type-III magnetic space groups. *Physical Review B*, **2022**, 105,	3.3	2
21	Fragile topologically protected perfect reflection for acoustic waves. *Physical Review Research*, **2020**, 2,	3.9	2
20	Observation of Topological Edge States on □BiBr Nanowires Grown on TiSe Substrates. *Journal of Physical Chemistry Letters*, **2021**, 12, 10465-10471	6.4	2
19	Observation of Nodal-Line Plasmons in ZrSiS. *Physical Review Letters*, **2021**, 127, 186802	7.4	2
18	The sensitivity determination of energetic materials from laser spark spectrometry based on physical-parameter-corrected statistical methods. *Journal of Analytical Atomic Spectrometry*,	3.7	2
17	Twofold symmetry of c-axis resistivity in topological kagome superconductor CsV3Sb5 with in-plane rotating magnetic field		2
16	Tailoring Dzyaloshinskii-Moriya interaction in a transition metal dichalcogenide by dual-intercalation. *Nature Communications*, **2021**, 12, 3639	17.4	2
15	Extraction of state-resolved information from systems with a fractional number of electrons within the framework of time-dependent density functional theory. *Journal of Chemical Physics*, **2016**, 145, 114104	3.0	2
14	Crystal chirality magneto-optical effects in collinear antiferromagnets. *Physical Review B*, **2021**, 104,	3.3	2
13	Intermediate anomalous Hall states induced by noncollinear spin structure in the magnetic topological insulator MnBi2Te4. *Physical Review B*, **2021**, 104,	3.3	2
12	Electron-phonon coupling in the charge density wave state of CsV3Sb5. *Physical Review B*, **2022**, 105,	3.3	2
11	Core hole effect on topological band order in cubic semiconductors: A first-principles study. *Europhysics Letters*, **2014**, 106, 27008	1.6	1
10	No observation of chiral flux current in the topological kagome metal CsV3Sb5. *Physical Review B*, **2022**, 105,	3.3	1
9	d+id? Chiral Superconductivity in Bilayer Silicene		1
8	Carrier Injection and Manipulation of Charge-Density Wave in Kagome Superconductor CsV3Sb5. *Physical Review X*, **2022**, 12,	9.1	1
7	Linear magnetization dependence and large intrinsic anomalous Hall effect in Fe78Si9B13 metallic glasses. *Physical Review B*, **2021**, 104,	3.3	1
6	Controllable epitaxy of quasi-one-dimensional topological insulator □Bi4Br4 for the application of saturable absorber. *Applied Physics Letters*, **2022**, 120, 093103	3.4	1

5	Trends of the macroscopic behaviors of energetic compounds: insights from first-principles calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 24034-24041	3.6	0
4	Pressure-induced novel nitrogen-rich aluminum nitrides: AlN, AlN and AlN with polymeric nitrogen chains and rings. *Physical Chemistry Chemical Physics*, **2021**, 23, 12350-12359	3.6	0
3	Controllable Growth of □and □Antimonene by Interfacial Strain. *Journal of Physical Chemistry C*, **2022**, 126, 5022-5027	3.8	0
2	Quasi-one-dimensional topological material Bi4X4(X=Br,I). *Advances in Physics: X*, **2022**, 7,	5.1	0
1	Memristive Crossbar Arrays for Storage and Computing Applications. *Advanced Intelligent Systems*, **2021**, 3, 2170065	6	