Chao Cao

List of Publications by Year
in descending order

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		126907	168389
110	3,381	33	53
papers	citations	h-index	g-index

111	111	111	4598
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	WannSymm: A symmetry analysis code for Wannier orbitals. Computer Physics Communications, 2022, 271, 108196.	7.5	22
2	Pressure-induced concomitant topological and metal-insulator quantum phase transitions in Ce3Pd3Bi4. Npj Quantum Materials, 2022, 7, .	5.2	2
3	Superconductivity with the enhanced upper critical field in the Pt-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CuRh</mml:mi><mml:mn>2</mml:mn></ spinel. Physical Review B, 2022, 105, .	3.2	4
4	Electronic structure and open-orbit Fermi surface topology in isostructural semimetals NbAs2 and W2As3 with extremely large magnetoresistance. Applied Physics Letters, 2022, 120, .	3.3	5
5	Manipulation of the ferromagnetic ordering in magnetic semiconductor (La,Ca)(Zn,Mn)AsO by chemical pressure. Journal of Magnetism and Magnetic Materials, 2022, 554, 169276.	2.3	2
6	Consecutive topological phase transitions and colossal magnetoresistance in a magnetic topological semimetal. Npj Quantum Materials, 2022, 7, .	5.2	10
7	Superconductivity in the nodal-line compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>3</mml:mn></ Physical Review Research, 2022, 4, .	3.6	4
8	Microscopic theory of superconducting phase diagram in infinite-layer nickelates. Physical Review B, 2022, 106, .	3.2	11
9	Anisotropic gapping of topological Weyl rings in the charge-density-wave superconductor In TaSe2. Science Bulletin, 2021, 66, 243-249.	9.0	11
10	Doping dependence of electronic structure of infinite-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>NdNiO</mml:mi></mml:mrow><mml:mn>2< Physical Review B, 2021, 103, .	3.2	24
11	Growth, electronic structure and superconductivity of ultrathin epitaxial CoSi2 films. Journal of Physics Condensed Matter, 2021, 33, 155501.	1.8	1
12	Tuning Rashba effect, band inversion, and spin-charge conversion of Janus <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>X</mml:mi><mml:msub><mml:mi>Sn2</mml:mi><mml:mn>4</mml:mn><mml:mn monolayers via an external field. Physical Review B, 2021, 103, .	3.2	48
13	Strain-dependent optical properties of the novel monolayer group-IV dichalcogenides SiS₂ semiconductor: a first-principles study. Nanotechnology, 2021, 32, 235201.	2.6	6
14	Bandwidth-control orbital-selective delocalization of 4f electrons in epitaxial Ce films. Nature Communications, 2021, 12, 2520.	12.8	17
15	Anisotropic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>c</mml:mi><mml:mo>â^'</mml:mo><mml:mi>f</mml:mi></mml:math> Hybridization in the Ferromagnetic Quantum Critical Metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CeRh</mml:mi></mml:mrow><mml:mrow><mml:mn>6</mml:mn></ Physical Review Letters, 2021, 126, 216406.	7.8	23
16	Coexistence of superconductivity and antiferromagentic order in Er2O2Bi with anti-ThCr2Si2 structure. Frontiers of Physics, 2021, 16, 1.	5.0	4
17	Intraband Elliott-Yafet Contribution and Stoner Ferromagnetism in Janus <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">P</mml:mi><mml:msub><mml:mi>A</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>As</mml:mi></		

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19	Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor CeCu2Si2. Physical Review Letters, 2021, 127, 067002.	7.8	17
20	Nodeless superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Lu</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mn>5</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> with broken time reversal symmetry. Physical Review B, 2021, 103, .	3.2	6
21	Charge density wave and weak Kondo effect in a Dirac semimetal CeSbTe. Science China: Physics, Mechanics and Astronomy, 2021, 64, 1.	5.1	16
22	Interfacial electron-phonon coupling and quantum confinement in ultrathin Yb films on graphite. Physical Review B, 2021, 104, .	3.2	1
23	Shubnikovâ€“de Haas oscillations and electronic structure in the Dirac semimetal SrAgAs. Physical Review B, 2021, 104, .	3.2	2
24	Intense d-p Hybridization Induced a Vast SHG Response Disparity between Tetrahedral Vanadates and Arsenates. Journal of Physical Chemistry C, 2020, 124, 24949-24956.	3.1	8
25	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. Physical Review Letters, 2020, 125, 187402.	7.8	94
26	Enhanced anisotropic superconductivity in the topological nodal-line semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> Physical Review B, 2020, 102, .	3.2	8
27	Electron-phonon coupling and nontrivial band topology in noncentrosymmetric superconductors LaNiSi, LaPtSi, and LaPtGe. Physical Review B, 2020, 101, .	3.2	16
28	Coexistence of nontrivial topological properties and strong ferromagnetic fluctuations in quasi-one-dimensional A2Cr3As3. Npj Computational Materials, 2020, 6, .	8.7	19
29	PrBi: Topology meets quadrupolar degrees of freedom. Physical Review B, 2020, 101, .	3.2	7
30	CaPtAs: A new noncentrosymmetric superconductor. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	5.1	26
31	From Trivial Kondo Insulator Ce3Pt3Bi4 to Topological Nodal-Line Semimetal Ce3Pd3Bi4. Physical Review Letters, 2020, 124, 166403.	7.8	19
32	Giant anomalous Nernst effect in the magnetic Weyl semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2020, 4, .	2.4	68
33	Prediction of spin polarized Fermi arcs in quasiparticle interference in CeBi. Physical Review B, 2020, 102, .	3.2	7
34	Large Fermi surface expansion through anisotropic mixing of conduction and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> electrons in the semimetallic Kondo lattice CeBi. Physical Review B, 2019, 100, .	3.2	12
35	Probing the origin of extreme magnetoresistance in Pr/Sm mono-antimonides/bismuthides. Physical Review B, 2019, 99, .	3.2	12
36	Large magnetoresistance and large magnetothermopower effect in the Dirac material EuMn_{0.8}Sb₂. Journal of Physics Condensed Matter, 2019, 31, 185701.	1.8	6

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37	Unique crystal field splitting and multiband RKKY interactions in Ni-doped EuRbFe4As4. Communications Physics, 2019, 2, .	5.3	17
38	Lifshitz transition and nontrivial H-doping effect in the Cr-based superconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">KCr</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">As</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>. Physical Review B, 2019, 100, .	3.2	17
39	Angle-dependent magnetoresistance and its implications for Lifshitz transition in W2As3. Npj Quantum Materials, 2019, 4, .	5.2	11
40	Optical signatures of Dirac nodal lines in NbAs ₂. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1168-1173.	7.1	60
41	Pressure induced superconductivity bordering a charge-density-wave state in NbTe4 with strong spin-orbit coupling. Scientific Reports, 2018, 8, 6298.	3.3	21
42	Evidence for Weyl fermions in a canonical heavy-fermion semimetal YbPtBi. Nature Communications, 2018, 9, 4622.	12.8	62
43	Quantum transport in a compensated semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">W</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>As</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> with nontrivial <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Z</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> indices. Physical Review B, 2018, 98, .	3.2	8
44	Tunable electronic structure and topological properties of LnPn (Ln=Ce, Pr, Sm, Gd, Yb; Pn=Sb, Bi). Communications Physics, 2018, 1, .	5.3	37
45	Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. Journal of the American Chemical Society, 2018, 140, 10726-10733.	13.7	127
46	Tunable electronic structure and surface states in rare-earth monobismuthides with partially filled <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> shell. Physical Review B, 2018, 98, .	3.2	31
47	Kondo behavior and metamagnetic phase transition in the heavy-fermion compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">CeBi</mml:mi><mml:mn mathvariant="bold">2</mml:mn></mml:msub></mml:math>. Physical Review B, 2018, 97, .	3.2	9
48	Large magnetoresistance and superconductivity in Î±-gallium single crystals. Npj Quantum Materials, 2018, 3, .	5.2	16
49	Theory for superconductivity in alkali chromium arsenides A2Cr3As3 (A = K, Rb, Cs). Science Bulletin, 2017, 62, 208-211.	9.0	40
50	The atomic size effect on hybrid inorganicâ€“organic perovskite CH₃NH₃BI₃ (B = Pb, Sn) from first-principles study. Modern Physics Letters B, 2017, 31, 1750139.	1.9	2
51	Electronic structure and topological properties of centrosymmetric MoAs2/WAs2 from first principles. Scientific Reports, 2017, 7, 10491.	3.3	6
52	Strain and electric field tunable electronic structure of buckled bismuthene. RSC Advances, 2017, 7, 39546-39555.	3.6	53
53	Magnetoresistance and robust resistivity plateau in MoAs2. Scientific Reports, 2017, 7, 15669.	3.3	25
54	Possible Weyl fermions in the magnetic Kondo system CeSb. Npj Quantum Materials, 2017, 2, .	5.2	55

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55	Emerging novel electronic structure in hydrogen-Arsenene-halogen nanosheets: A computational study. Scientific Reports, 2017, 7, 4773.	3.3	9
56	Electronegativity explanation on the efficiency-enhancing mechanism of the hybrid inorganicâ€“organic perovskite ABX ₃ from first-principles study. Chinese Physics B, 2016, 25, 027104.	1.4	21
57	Cadmium and lithium doping in silver orthophosphate: An ab initio study. Scientific Reports, 2016, 6, 32574.	3.3	2
58	Two superconducting domes separated by a possible Lifshitz transition in LaFeAs1â^'xPxO. Journal of Applied Physics, 2016, 119, 083903.	2.5	7
59	Superconductivity in a new layered nickel selenide CsNi₂Se₂. Superconductor Science and Technology, 2016, 29, 045008.	3.5	7
60	The electronic structure of graphene tuned by hexagonal boron nitrogen layers: Semimetalâ€“semiconductor transition. Modern Physics Letters B, 2016, 30, 1650191.	1.9	6
61	Resistivity plateau and negative magnetoresistance in the topological semimetal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TaSb</mml:mi><mml:mn>2</mml:mn></mml:msub></ Physical Review B, 2016, 94,	3.2	88
62	Electronic structures of transition metal dipnictides<mml:math		

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73	Electronic phase diagram in a new BiS₂-based Sr_{1â”x}La_xFBiS₂system. Superconductor Science and Technology, 2014, 27, 035009.	3.5	25
74	Impact of lattice distortion and electron doping on Î±-MoO3 electronic structure. Scientific Reports, 2014, 4, 7131.	3.3	107
75	The origin of the high work function of chlorinated indium tin oxide. NPG Asia Materials, 2013, 5, e57-e57.	7.9	41
76	Effect of selenium doping on the superconductivity of Nb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow		

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91	Accurate projected augmented wave datasets for BaFe₂As₂. New Journal of Physics, 2010, 12, 123029.	2.9	3
92	Manipulating Iâ^'V Characteristics of a Molecular Switch with Chemical Modifications. Journal of Physical Chemistry C, 2010, 114, 1655-1662.	3.1	13
93	Electronic structure of substitutionally Mn-doped graphene. New Journal of Physics, 2010, 12, 063020.	2.9	83
94	Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures. Physical Review B, 2010, 81, .	3.2	234
95	Effects of cobalt doping and three-dimensionality in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2009, 80, .	3.2	54
96	Nonequilibrium Greenâ€™s function study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pd</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msu carbon nanotubes as hydrogen sensors. Physical Review B, 2009, 79, .	3.2	19
97	Molecular Dynamics Simulations of Au Penetration through Alkanethiol Monolayers on the Au(111) Surface. Journal of Physical Chemistry C, 2009, 113, 6360-6366.	3.1	7
98	Finding stable Î±-quartz (0001) surface structures via simulations. Applied Physics Letters, 2008, 93, .	3.3	42
99	Proximity of antiferromagnetism and superconductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaFeAsO</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</m Effective Hamiltonian fromab initiostudies. Physical Review B, 2008, 77, .	3.2	245
100	Determining gap nodal structures in Fe-based superconductors: Theory of the angle dependence of the low-temperature specific heat in an applied magnetic field. Physical Review B, 2008, 77, .	3.2	47
101	First-principles simulations of dissociated and molecular<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>adsorption on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">Pd</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>-cluster-functionalized	3.2	8
102	Predictive first-principles simulations of strain-induced phenomena at water-silica nanotube interfaces. Journal of Chemical Physics, 2008, 129, 011101.	3.0	7
103	Strongly Correlated Electrons in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo stretchy="false">[</mml:mo><mml:mi>Ni</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>hmp</mml:mi><mml:mo stretchy="false">)</mml:mo><mml:mo stretchy="false">(</mml:mo><mml:mi>R</mml:mi><mml:mi>OH</mml:mi><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	7.8	40
104	stretchy="false">]</mml:mo><mml:mn>4</mml:mn></mml:msub></mml:math>Single Molecule Magnet: First-principles determination of the effects of intermolecular interactions on the electronic transport through molecular monolayers. Physical Review B, 2008, 78, .	3.2	12
105	Effects of strain and defects on the electron conductance of metallic carbon nanotubes. Physical Review B, 2007, 75, .	3.2	36
106	Fracture, water dissociation, and proton conduction in SiO2 nanochains. Journal of Chemical Physics, 2007, 126, 211101.	3.0	18
107	PUPIL: A systematic approach to software integration in multi-scale simulations. Computer Physics Communications, 2007, 177, 265-279.	7.5	21
108	Environment dependent dynamic charge potential for silica: Application to nanoscale silica structures. Chemical Physics Letters, 2007, 437, 92-98.	2.6	8

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109	Quantum, classical, and multi-scale simulation of silicaâ€“water interaction: molecules, clusters, and extended systems. Journal of Computer-Aided Materials Design, 2006, 13, 161-183.	0.7	11
110	From cluster to bulk: Size dependent energetics of silica and silica-water interaction. Journal of Chemical Physics, 2006, 124, 024722.	3.0	13