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	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</mml:mn> Effective Hamiltonian fromab initiostudies. Physical Review B, 2008, 77, .	3.2	245
2	Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures. Physical Review B, 2010, 81, .	3.2	234
3	Light non-metallic atom (B, N, O and F)-doped graphene: a first-principles study. Nanotechnology, 2010, 21, 505202.	2.6	207
4	Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. Journal of the American Chemical Society, 2018, 140, 10726-10733.	13.7	127
5	Impact of lattice distortion and electron doping on Î±-MoO3 electronic structure. Scientific Reports, 2014, 4, 7131.	3.3	107
6	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. Physical Review Letters, 2020, 125, 187402.	7.8	94
7	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
8	Electronic structure of substitutionally Mn-doped graphene. New Journal of Physics, 2010, 12, 063020.	2.9	83
9	Electronic structure of quasi-one-dimensional superconductor K2Cr3As3 from first-principles calculations. Scientific Reports, 2015, 5, 16054.	3.3	72
10	Block Spin Ground State and Three-Dimensionality of(K,Tl)yFe1.6Se2. Physical Review Letters, 2011, 107, 056401.	7.8	71
11	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:mr mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2020, 4, .	2.4	68
12	Evidence for Weyl fermions in a canonical heavy-fermion semimetal YbPtBi. Nature Communications, 2018, 9, 4622.	12.8	62
13	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
14	Metal-terminated graphene nanoribbons. Physical Review B, 2010, 82, .	3.2	58
15	Unexpected electronic structure of the alloyed and doped arsenene sheets: First-Principles calculations. Scientific Reports, 2016, 6, 29114.	3.3	58
16	Possible Weyl fermions in the magnetic Kondo system CeSb. Npj Quantum Materials, 2017, 2, .	5.2	55
17	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:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 80, .	3.2	54
18	Strain and electric field tunable electronic structure of buckled bismuthene. RSC Advances, 2017, 7, 39546-39555.	3.6	53

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19	Diastereomeric structures of transition metal dipnictides<mml:math		

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37	CaPtAs: A new noncentrosymmetric superconductor. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	5.1	26
38	Electronic phase diagram in a new BiS₂-based Sr_{1â^'x}La_xFBiS₂system. Superconductor Science and Technology, 2014, 27, 035009.	3.5	25
39	Magnetoresistance and robust resistivity plateau in MoAs2. Scientific Reports, 2017, 7, 15669.	3.3	25
40	Predicting Global Minimum in Complex Beryllium Borate System for Deep-ultraviolet Functional Optical Applications. Scientific Reports, 2016, 6, 34839.	3.3	24
41	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</mml:mn> Physical Review B, 2021, 103, .	3.2	24
42	Controllable spin-orbit coupling and its influence on the upper critical field in the chemically doped quasi-one-dimensional<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Nb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">PdS</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math>superconductor. Physical Review B, 2014, 90, .	3.2	23
43	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
44	WannSymm: A symmetry analysis code for Wannier orbitals. Computer Physics Communications, 2022, 271, 108196.	7.5	22
45	PUPIL: A systematic approach to software integration in multi-scale simulations. Computer Physics Communications, 2007, 177, 265-279.	7.5	21
46	Correlation-Induced Self-Doping in the Iron-Pnictide Superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Ba</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Ti</mml:mi><mml:mn mathvariant="normal">O</mml:mi></mml:math>. Physical Review Letters, 2014, 113, 266407.	7.8	21
47	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
48	Pressure induced superconductivity bordering a charge-density-wave state in NbTe4 with strong spin-orbit coupling. Scientific Reports, 2018, 8, 6298.	3.3	21
49	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:mu carbon nanotubes as hydrogen sensors. Physical Review B, 2009, 79, .	3.2	19
50	Perfect spin-filtering and giant magnetoresistance with Fe-terminated graphene nanoribbon. Applied Physics Letters, 2011, 99, .	3.3	19
51	Coexistence of nontrivial topological properties and strong ferromagnetic fluctuations in quasi-one-dimensional A2Cr3As3. Npj Computational Materials, 2020, 6, .	8.7	19
52	From Trivial Kondo Insulator Ce3Pt3Bi4 to Topological Nodal-Line Semimetal Ce3Pd3Bi4. Physical Review Letters, 2020, 124, 166403.	7.8	19
53	Fracture, water dissociation, and proton conduction in SiO2 nanochains. Journal of Chemical Physics, 2007, 126, 211101.	3.0	18
54	Reduced dimensionality and magnetic frustration in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>KCr</mml:mi><mml:mn>3</mml:mn></mml:mrow><mml:mn></mml Physical Review B, 2015, 92, .	3.2	17

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55	Unique crystal field splitting and multiband RKKY interactions in Ni-doped EuRbFe4As4. Communications Physics, 2019, 2, .	5.3	17
56	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
57	Bandwidth-control orbital-selective delocalization of 4f electrons in epitaxial Ce films. Nature Communications, 2021, 12, 2520.	12.8	17
58	Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor CeCu2Si2. Physical Review Letters, 2021, 127, 067002.	7.8	17
59	Large magnetoresistance and superconductivity in Î±-gallium single crystals. Npj Quantum Materials, 2018, 3, .	5.2	16
60	Electron-phonon coupling and nontrivial band topology in noncentrosymmetric superconductors LaNiSi, LaPtSi, and LaPtGe. Physical Review B, 2020, 101, .	3.2	16
61	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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73	Angle-dependent magnetoresistance and its implications for Lifshitz transition in W2As3. Npj Quantum Materials, 2019, 4, .	5.2	11
74	Anisotropic gapping of topological Weyl rings in the charge-density-wave superconductor In TaSe2. Science Bulletin, 2021, 66, 243-249.	9.0	11
75	Microscopic theory of superconducting phase diagram in infinite-layer nickelates. Physical Review B, 2022, 106, .	3.2	11
76	Consecutive topological phase transitions and colossal magnetoresistance in a magnetic topological semimetal. Npj Quantum Materials, 2022, 7, .	5.2	10
77	Magnetic properties and magnetic phase diagram in the Co-rich side of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>L</mml:mi></mml:math>Co<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>Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>	3.2	9
78	Emerging novel electronic structure in hydrogen-Arsenene-halogen nanosheets: A computational study. Scientific Reports, 2017, 7, 4773.	3.3	9
79	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
80	Environment dependent dynamic charge potential for silica: Application to nanoscale silica structures. Chemical Physics Letters, 2007, 437, 92-98.	2.6	8
81	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
82	Electronic structure of vacancy-ordered iron-selenide K0.5Fe1.75Se2. Physical Review B, 2013, 87, .	3.2	8
83	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></	3.2	8
84	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
85	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
86	Predictive first-principles simulations of strain-induced phenomena at water-silica nanotube interfaces. Journal of Chemical Physics, 2008, 129, 011101.	3.0	7
87	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
88	Two superconducting domes separated by a possible Lifshitz transition in LaFeAs1â^’xPxO. Journal of Applied Physics, 2016, 119, 083903.	2.5	7
89	Superconductivity in a new layered nickel selenide CsNi₂Se₂. Superconductor Science and Technology, 2016, 29, 045008.	3.5	7
90	PrBi: Topology meets quadrupolar degrees of freedom. Physical Review B, 2020, 101, .	3.2	7

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91	Prediction of spin polarized Fermi arcs in quasiparticle interference in CeBi. Physical Review B, 2020, 102, .	3.2	7
92	The electronic properties of impurities (N, C, F, Cl and S) in Ag3PO4: A hybrid functional method study. Scientific Reports, 2015, 5, 12750.	3.3	6
93	The electronic structure of graphene tuned by hexagonal boron nitrogen layers: Semimetalâ€“semiconductor transition. Modern Physics Letters B, 2016, 30, 1650191.	1.9	6
94	Electronic structure and topological properties of centrosymmetric MoAs2/WAs2 from first principles. Scientific Reports, 2017, 7, 10491.	3.3	6
95	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
96	Strain-dependent optical properties of the novel monolayer group-IV dichalcogenides SiS₂ semiconductor: a first-principles study. Nanotechnology, 2021, 32, 235201.	2.6	6
97	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:msub><mml:mn>5</mml:n with broken time reversal symmetry. Physical Review B, 2021, 103, .	3.2	6
98	Block spin magnetism and metal-insulator transition in a two-dimensional Hubbard model with perfect vacancy superstructure. Physical Review B, 2011, 83, .	3.2	5
99	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
100	Coexistence of superconductivity and antiferromagentic order in Er2O2Bi with anti-ThCr2Si2 structure. Frontiers of Physics, 2021, 16, 1.	5.0	4
101	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
102	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></mml:m Physical Review Research, 2022, 4, .	3.6	4
103	Accurate projected augmented wave datasets for BaFe₂As₂. New Journal of Physics, 2010, 12, 123029.	2.9	3
104	Cadmium and lithium doping in silver orthophosphate: An ab initio study. Scientific Reports, 2016, 6, 32574.	3.3	2
105	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
106	Shubnikovâ€“de Haas oscillations and electronic structure in the Dirac semimetal SrAgAs. Physical Review B, 2021, 104, .	3.2	2
107	Pressure-induced concomitant topological and metal-insulator quantum phase transitions in Ce3Pd3Bi4. Npj Quantum Materials, 2022, 7, .	5.2	2
108	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

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109	Growth, electronic structure and superconductivity of ultrathin epitaxial CoSi2 films. Journal of Physics Condensed Matter, 2021, 33, 155501.	1.8	1
110	Interfacial electron-phonon coupling and quantum confinement in ultrathin Yb films on graphite. Physical Review B, 2021, 104, .	3.2	1