Chao Cao

List of Publications by Year in Descending Order

100 papers	2,440 citations	28 h-index	46 g-index
111 ext. papers	2,934 ext. citations	4.5 avg, IF	5.26 L-index

#	Paper	IF	Citations
100	WannSymm: A symmetry analysis code for Wannier orbitals. *Computer Physics Communications*, **2022**, 271, 108196	4.2	1
99	Electronic structure and open-orbit Fermi surface topology in isostructural semimetals NbAs2 and W2As3 with extremely large magnetoresistance. *Applied Physics Letters*, **2022**, 120, 123101	3.4	1
98	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	2.8	
97	Strain-dependent optical properties of the novel monolayer group-IV dichalcogenides SiS2 semiconductor: A first-principles study. *Nanotechnology*, **2021**,	3.4	1
96	Bandwidth-control orbital-selective delocalization of 4f electrons in epitaxial Ce films. *Nature Communications*, **2021**, 12, 2520	17.4	1
95	Anisotropic c-f Hybridization in the Ferromagnetic Quantum Critical Metal CeRh_{6}Ge_{4}. *Physical Review Letters*, **2021**, 126, 216406	7.4	5
94	Coexistence of superconductivity and antiferromagentic order in Er2O2Bi with anti-ThCr2Si2 structure. *Frontiers of Physics*, **2021**, 16, 1	3.7	2
93	Anisotropic gapping of topological Weyl rings in the charge-density-wave superconductor In TaSe2. *Science Bulletin*, **2021**, 66, 243-249	10.6	6
92	Doping dependence of electronic structure of infinite-layer NdNiO2. *Physical Review B*, **2021**, 103,	3.3	10
91	Tuning Rashba effect, band inversion, and spin-charge conversion of Janus XSn2Y monolayers via an external field. *Physical Review B*, **2021**, 103,	3.3	12
90	Localized 4f-electrons in the quantum critical heavy fermion ferromagnet CeRh6Ge4. *Science Bulletin*, **2021**, 66, 1389-1394	10.6	5
89	Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor CeCu_{2}Si_{2}. *Physical Review Letters*, **2021**, 127, 067002	7.4	2
88	Charge density wave and weak Kondo effect in a Dirac semimetal CeSbTe. *Science China: Physics, Mechanics and Astronomy*, **2021**, 64, 1	3.6	4
87	Electron-phonon coupling and nontrivial band topology in noncentrosymmetric superconductors LaNiSi, LaPtSi, and LaPtGe. *Physical Review B*, **2020**, 101,	3.3	3
86	Coexistence of nontrivial topological properties and strong ferromagnetic fluctuations in quasi-one-dimensional A2Cr3As3. *Npj Computational Materials*, **2020**, 6,	10.9	10
85	PrBi: Topology meets quadrupolar degrees of freedom. *Physical Review B*, **2020**, 101,	3.3	2
84	CaPtAs: A new noncentrosymmetric superconductor. *Science China: Physics, Mechanics and Astronomy*, **2020**, 63, 1	3.6	8

83	Giant anomalous Nernst effect in the magnetic Weyl semimetal Co3Sn2S2. *Physical Review Materials*, **2020**, 4,	3.2	26
82	Prediction of spin polarized Fermi arcs in quasiparticle interference in CeBi. *Physical Review B*, **2020**, 102,	3.3	3
81	Intense d-p Hybridization Induced a Vast SHG Response Disparity between Tetrahedral Vanadates and Arsenates. *Journal of Physical Chemistry C*, **2020**, 124, 24949-24956	3.8	5
80	Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. *Physical Review Letters*, **2020**, 125, 187402	7.4	23
79	Enhanced anisotropic superconductivity in the topological nodal-line semimetal InxTaS2. *Physical Review B*, **2020**, 102,	3.3	4
78	From Trivial Kondo Insulator Ce_{3}Pt_{3}Bi_{4} to Topological Nodal-Line Semimetal Ce_{3}Pd_{3}Bi_{4}. *Physical Review Letters*, **2020**, 124, 166403	7.4	5
77	Large Fermi surface expansion through anisotropic mixing of conduction and f electrons in the semimetallic Kondo lattice CeBi. *Physical Review B*, **2019**, 100,	3.3	5
76	Probing the origin of extreme magnetoresistance in Pr/Sm mono-antimonides/bismuthides. *Physical Review B*, **2019**, 99,	3.3	4
75	Large magnetoresistance and large magnetothermopower effect in the Dirac material EuMnSb. *Journal of Physics Condensed Matter*, **2019**, 31, 185701	1.8	2
74	Unique crystal field splitting and multiband RKKY interactions in Ni-doped EuRbFe4As4. *Communications Physics*, **2019**, 2,	5.4	13
73	Lifshitz transition and nontrivial H-doping effect in the Cr-based superconductor KCr3As3Hx. *Physical Review B*, **2019**, 100,	3.3	10
72	Angle-dependent magnetoresistance and its implications for Lifshitz transition in W2As3. *Npj Quantum Materials*, **2019**, 4,	5	3
71	Optical signatures of Dirac nodal lines in NbAs. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 1168-1173	11.5	35
70	Pressure induced superconductivity bordering a charge-density-wave state in NbTe with strong spin-orbit coupling. *Scientific Reports*, **2018**, 8, 6298	4.9	11
69	Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. *Journal of the American Chemical Society*, **2018**, 140, 10726-10733	16.4	76
68	Tunable electronic structure and surface states in rare-earth monobismuthides with partially filled f shell. *Physical Review B*, **2018**, 98,	3.3	16
67	Kondo behavior and metamagnetic phase transition in the heavy-fermion compound CeBi2. *Physical Review B*, **2018**, 97,	3.3	3
66	Large magnetoresistance and superconductivity in gallium single crystals. *Npj Quantum Materials*, **2018**, 3,	5	10

65	Evidence for Weyl fermions in a canonical heavy-fermion semimetal YbPtBi. *Nature Communications*, **2018**, 9, 4622	17.4	33
64	Quantum transport in a compensated semimetal W2As3 with nontrivial Z2 indices. *Physical Review B*, **2018**, 98,	3.3	7
63	Tunable electronic structure and topological properties of LnPn (Ln=Ce, Pr, Sm, Gd, Yb; Pn=Sb, Bi). *Communications Physics*, **2018**, 1,	5.4	16
62	Theory for superconductivity in alkali chromium arsenides A2Cr3As3 (A = K, Rb, Cs). *Science Bulletin*, **2017**, 62, 208-211	10.6	31
61	The atomic size effect on hybrid inorganic□rganic perovskite CH3NH3BI3 (B = Pb, Sn) from first-principles study. *Modern Physics Letters B*, **2017**, 31, 1750139	1.6	2
60	Electronic structure and topological properties of centrosymmetric MoAs/WAs from first principles. *Scientific Reports*, **2017**, 7, 10491	4.9	3
59	Strain and electric field tunable electronic structure of buckled bismuthene. *RSC Advances*, **2017**, 7, 39546-39555	3.7	41
58	Magnetoresistance and robust resistivity plateau in MoAs. *Scientific Reports*, **2017**, 7, 15669	4.9	20
57	Possible Weyl fermions in the magnetic Kondo system CeSb. *Npj Quantum Materials*, **2017**, 2,	5	38
56	Emerging novel electronic structure in hydrogen-Arsenene-halogen nanosheets: A computational study. *Scientific Reports*, **2017**, 7, 4773	4.9	9
55	Resistivity plateau and negative magnetoresistance in the topological semimetal TaSb2. *Physical Review B*, **2016**, 94,	3.3	61
54	Electronic structures of transition metal dipnictides XPn2 (X=Ta, Nb; Pn=P, As, Sb). *Physical Review B*, **2016**, 93,	3.3	35
53	Unexpected electronic structure of the alloyed and doped arsenene sheets: First-Principles calculations. *Scientific Reports*, **2016**, 6, 29114	4.9	49
52	Predicting Global Minimum in Complex Beryllium Borate System for Deep-ultraviolet Functional Optical Applications. *Scientific Reports*, **2016**, 6, 34839	4.9	20
51	Electronegativity explanation on the efficiency-enhancing mechanism of the hybrid inorganic□rganic perovskite ABX 3 from first-principles study. *Chinese Physics B*, **2016**, 25, 027104	1.2	15
50	Cadmium and lithium doping in silver orthophosphate: An ab initio study. *Scientific Reports*, **2016**, 6, 32574	4.9	1
49	Two superconducting domes separated by a possible Lifshitz transition in LaFeAs1□PxO. *Journal of Applied Physics*, **2016**, 119, 083903	2.5	4
48	Superconductivity in a new layered nickel selenide CsNi2Se2. *Superconductor Science and Technology*, **2016**, 29, 045008	3.1	5

47	The electronic structure of graphene tuned by hexagonal boron nitrogen layers: Semimetal□emiconductor transition. *Modern Physics Letters B*, **2016**, 30, 1650191	1.6	4
46	Reduced dimensionality and magnetic frustration in KCr3As3. *Physical Review B*, **2015**, 92,	3.3	15
45	Electronic structure of quasi-one-dimensional superconductor K2Cr3As3 from first-principles calculations. *Scientific Reports*, **2015**, 5, 16054	4.9	59
44	The electronic properties of impurities (N, C, F, Cl, and S) in Ag3PO4: A hybrid functional method study. *Scientific Reports*, **2015**, 5, 12750	4.9	6
43	Upward Curvature of the Upper Critical Field and the V-Shaped Pressure Dependence of T c in the Noncentrosymmetric Superconductor PbTaSe2. *Journal of Superconductivity and Novel Magnetism*, **2015**, 28, 3173-3178	1.5	12
42	Impact of lattice distortion and electron doping on □MoO3 electronic structure. *Scientific Reports*, **2014**, 4, 7131	4.9	75
41	Electronic phase diagram in a new BiS2-based Sr1□LaxFBiS2system. *Superconductor Science and Technology*, **2014**, 27, 035009	3.1	22
40	Correlation-induced self-doping in the iron-pnictide superconductor Ba2Ti2Fe2As4O. *Physical Review Letters*, **2014**, 113, 266407	7.4	19
39	Controllable spin-orbit coupling and its influence on the upper critical field in the chemically doped quasi-one-dimensional Nb2PdS5 superconductor. *Physical Review B*, **2014**, 90,	3.3	16
38	Visualization of atomic-scale phenomena in superconductors: Application to FeSe. *Physical Review B* , **2014**, 90,	3.3	28
37	Electronic nematicity revealed by torque magnetometry in EuFe2(As1□Px)2. *Physical Review B*, **2014**, 89,	3.3	11
36	The origin of the high work function of chlorinated indium tin oxide. *NPG Asia Materials*, **2013**, 5, e57-e57	10.3	28
35	Effect of selenium doping on the superconductivity of Nb2Pd(S1□Sex)5. *Physical Review B*, **2013**, 88,	3.3	31
34	Superconductivity, charge- or spin-density wave, and metal-nonmetal transition in BaTi2(Sb1□Bix)2O. *Physical Review B*, **2013**, 87,	3.3	33
33	Li2RhO3: A spin-glassy relativistic Mott insulator. *Physical Review B*, **2013**, 87,	3.3	36
32	Electronic structure of vacancy-ordered iron-selenide K0.5Fe1.75Se2. *Physical Review B*, **2013**, 87,	3.3	7
31	K and Mn co-doped BaCd2As2: A hexagonal structured bulk diluted magnetic semiconductor with large magnetoresistance. *Journal of Applied Physics*, **2013**, 114, 223905	2.5	33
30	First-principles calculations of the electronic and phonon properties of APt3P (A = Ca, Sr, and La): Evidence for a charge-density-wave instability and a soft phonon. *Physical Review B*, **2012**, 86,	3.3	26

29	Magnetic phase diagram in the Co-rich side of the LCo1−xFexAsO (L = La, Sm) system. *Physical Review B*, **2012**, 86,	3.3	8
28	Block spin ground state and three-dimensionality of (K,Tl)(y)Fe(1.6)Se2. *Physical Review Letters*, **2011**, 107, 056401	7.4	65
27	OPAL: A multiscale multicenter simulation package based on MPI-2 protocol. *International Journal of Quantum Chemistry*, **2011**, 111, 4020-4029	2.1	5
26	Electronic structure and Mott localization of iron-deficient TlFe1.5Se2 with superstructures. *Physical Review B*, **2011**, 83,	3.3	27
25	Perfect spin-filtering and giant magnetoresistance with Fe-terminated graphene nanoribbon. *Applied Physics Letters*, **2011**, 99, 073110	3.4	18
24	Block spin magnetism and metal-insulator transition in a two-dimensional Hubbard model with perfect vacancy superstructure. *Physical Review B*, **2011**, 83,	3.3	5
23	Electronic Structure of KFe 2 Se 2 from First-Principles Calculations. *Chinese Physics Letters*, **2011**, 28, 057402	1.8	38
22	Metal-terminated graphene nanoribbons. *Physical Review B*, **2010**, 82,	3.3	50
21	Light non-metallic atom (B, N, O and F)-doped graphene: a first-principles study. *Nanotechnology*, **2010**, 21, 505202	3.4	184
20	Accurate projected augmented wave datasets for BaFe2As2. *New Journal of Physics*, **2010**, 12, 123029	2.9	2
19	Manipulating I–V Characteristics of a Molecular Switch with Chemical Modifications. *Journal of Physical Chemistry C*, **2010**, 114, 1655-1662	3.8	12
18	Electronic structure of substitutionally Mn-doped graphene. *New Journal of Physics*, **2010**, 12, 063020	2.9	75
17	Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures. *Physical Review B*, **2010**, 81,	3.3	217
16	Effects of cobalt doping and three-dimensionality in BaFe2As2. *Physical Review B*, **2009**, 80,	3.3	52
15	Nonequilibrium Green□ function study of Pd4-cluster-functionalized carbon nanotubes as hydrogen sensors. *Physical Review B*, **2009**, 79,	3.3	17
14	Molecular Dynamics Simulations of Au Penetration through Alkanethiol Monolayers on the Au(111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 6360-6366	3.8	7
13	Finding stable □quartz (0001) surface structures via simulations. *Applied Physics Letters*, **2008**, 93, 181911	3.4	35
12	Proximity of antiferromagnetism and superconductivity in LaFeAsO1−xFx: Effective Hamiltonian from ab initio studies. *Physical Review B*, **2008**, 77,	3.3	233

11	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,	3.3	44
10	First-principles simulations of dissociated and molecular H2 adsorption on Pd4-cluster-functionalized carbon nanotubes. *Physical Review B*, **2008**, 77,	3.3	8
9	Predictive first-principles simulations of strain-induced phenomena at water-silica nanotube interfaces. *Journal of Chemical Physics*, **2008**, 129, 011101	3.9	7
8	Strongly correlated electrons in the [Ni(hmp)(ROH)X]4 single molecule magnet: a DFT+U study. *Physical Review Letters*, **2008**, 100, 167206	7.4	35
7	First-principles determination of the effects of intermolecular interactions on the electronic transport through molecular monolayers. *Physical Review B*, **2008**, 78,	3.3	12
6	Fracture, water dissociation, and proton conduction in SiO2 nanochains. *Journal of Chemical Physics*, **2007**, 126, 211101	3.9	18
5	PUPIL: A systematic approach to software integration in multi-scale simulations. *Computer Physics Communications*, **2007**, 177, 265-279	4.2	20
4	Environment dependent dynamic charge potential for silica: Application to nanoscale silica structures. *Chemical Physics Letters*, **2007**, 437, 92-98	2.5	7
3	Effects of strain and defects on the electron conductance of metallic carbon nanotubes. *Physical Review B*, **2007**, 75,	3.3	34
2	From cluster to bulk: size dependent energetics of silica and silica-water interaction. *Journal of Chemical Physics*, **2006**, 124, 024722	3.9	13
1	Quantum, classical, and multi-scale simulation of silica–water interaction: molecules, clusters, and extended systems. *Journal of Computer-Aided Materials Design*, **2006**, 13, 161-183		11