# Chao Cao

## List of Publications by Citations



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|---|---|---|---|
| 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 | Proximity of antiferromagnetism and superconductivity in LaFeAsO1−xFx: Effective Hamiltonian from ab initio studies. *Physical Review B*, **2008**, 77, | 3.3 | 233 |
| 99 | Transition metal adatom and dimer adsorbed on graphene: Induced magnetization and electronic structures. *Physical Review B*, **2010**, 81, | 3.3 | 217 |
| 98 | Light non-metallic atom (B, N, O and F)-doped graphene: a first-principles study. *Nanotechnology*, **2010**, 21, 505202 | 3.4 | 184 |
| 97 | Module-Guided Design Scheme for Deep-Ultraviolet Nonlinear Optical Materials. *Journal of the American Chemical Society*, **2018**, 140, 10726-10733 | 16.4 | 76 |
| 96 | Impact of lattice distortion and electron doping on α-MoO3 electronic structure. *Scientific Reports*, **2014**, 4, 7131 | 4.9 | 75 |
| 95 | Electronic structure of substitutionally Mn-doped graphene. *New Journal of Physics*, **2010**, 12, 063020 | 2.9 | 75 |
| 94 | Block spin ground state and three-dimensionality of (K,Tl)(y)Fe(1.6)Se2. *Physical Review Letters*, **2011**, 107, 056401 | 7.4 | 65 |
| 93 | Resistivity plateau and negative magnetoresistance in the topological semimetal TaSb2. *Physical Review B*, **2016**, 94, | 3.3 | 61 |
| 92 | Electronic structure of quasi-one-dimensional superconductor K2Cr3As3 from first-principles calculations. *Scientific Reports*, **2015**, 5, 16054 | 4.9 | 59 |
| 91 | Effects of cobalt doping and three-dimensionality in BaFe2As2. *Physical Review B*, **2009**, 80, | 3.3 | 52 |
| 90 | Metal-terminated graphene nanoribbons. *Physical Review B*, **2010**, 82, | 3.3 | 50 |
| 89 | Unexpected electronic structure of the alloyed and doped arsenene sheets: First-Principles calculations. *Scientific Reports*, **2016**, 6, 29114 | 4.9 | 49 |
| 88 | 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 |
| 87 | Strain and electric field tunable electronic structure of buckled bismuthene. *RSC Advances*, **2017**, 7, 39546-39555 | 3.7 | 41 |
| 86 | Possible Weyl fermions in the magnetic Kondo system CeSb. *Npj Quantum Materials*, **2017**, 2, | 5 | 38 |
| 85 | Electronic Structure of KFe 2 Se 2 from First-Principles Calculations. *Chinese Physics Letters*, **2011**, 28, 057402 | 1.8 | 38 |
| 84 | Li2RhO3: A spin-glassy relativistic Mott insulator. *Physical Review B*, **2013**, 87, | 3.3 | 36 |

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|---|---|---|---|
| 83 | Electronic structures of transition metal dipnictides XPn2 (X=Ta, Nb; Pn=P, As, Sb). *Physical Review B*, **2016**, 93, | 3.3 | 35 |
| 82 | Finding stable □quartz (0001) surface structures via simulations. *Applied Physics Letters*, **2008**, 93, 181911 | 3.4 | 35 |
| 81 | 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 |
| 80 | 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 |
| 79 | Effects of strain and defects on the electron conductance of metallic carbon nanotubes. *Physical Review B*, **2007**, 75, | 3.3 | 34 |
| 78 | Superconductivity, charge- or spin-density wave, and metal-nonmetal transition in BaTi2(Sb1⊠Bix)2O. *Physical Review B*, **2013**, 87, | 3.3 | 33 |
| 77 | 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 |
| 76 | Evidence for Weyl fermions in a canonical heavy-fermion semimetal YbPtBi. *Nature Communications*, **2018**, 9, 4622 | 17.4 | 33 |
| 75 | Theory for superconductivity in alkali chromium arsenides A2Cr3As3 (A = K, Rb, Cs). *Science Bulletin*, **2017**, 62, 208-211 | 10.6 | 31 |
| 74 | Effect of selenium doping on the superconductivity of Nb2Pd(S1⊠Sex)5. *Physical Review B*, **2013**, 88, | 3.3 | 31 |
| 73 | The origin of the high work function of chlorinated indium tin oxide. *NPG Asia Materials*, **2013**, 5, e57-e57 | 10.3 | 28 |
| 72 | Visualization of atomic-scale phenomena in superconductors: Application to FeSe. *Physical Review B*, **2014**, 90, | 3.3 | 28 |
| 71 | Electronic structure and Mott localization of iron-deficient TlFe1.5Se2 with superstructures. *Physical Review B*, **2011**, 83, | 3.3 | 27 |
| 70 | 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 |
| 69 | Giant anomalous Nernst effect in the magnetic Weyl semimetal Co3Sn2S2. *Physical Review Materials*, **2020**, 4, | 3.2 | 26 |
| 68 | Second Harmonic Generation Susceptibilities from Symmetry Adapted Wannier Functions. *Physical Review Letters*, **2020**, 125, 187402 | 7.4 | 23 |
| 67 | Electronic phase diagram in a new BiS2-based Sr1⊠LaxFBiS2system. *Superconductor Science and Technology*, **2014**, 27, 035009 | 3.1 | 22 |
| 66 | Predicting Global Minimum in Complex Beryllium Borate System for Deep-ultraviolet Functional Optical Applications. *Scientific Reports*, **2016**, 6, 34839 | 4.9 | 20 |

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| 65 | Magnetoresistance and robust resistivity plateau in MoAs. *Scientific Reports*, **2017**, 7, 15669 | 4.9 | 20 |
| 64 | PUPIL: A systematic approach to software integration in multi-scale simulations. *Computer Physics Communications*, **2007**, 177, 265-279 | 4.2 | 20 |
| 63 | Correlation-induced self-doping in the iron-pnictide superconductor Ba2Ti2Fe2As4O. *Physical Review Letters*, **2014**, 113, 266407 | 7.4 | 19 |
| 62 | Perfect spin-filtering and giant magnetoresistance with Fe-terminated graphene nanoribbon. *Applied Physics Letters*, **2011**, 99, 073110 | 3.4 | 18 |
| 61 | Fracture, water dissociation, and proton conduction in SiO2 nanochains. *Journal of Chemical Physics*, **2007**, 126, 211101 | 3.9 | 18 |
| 60 | Nonequilibrium Green□ function study of Pd4-cluster-functionalized carbon nanotubes as hydrogen sensors. *Physical Review B*, **2009**, 79, | 3.3 | 17 |
| 59 | Tunable electronic structure and surface states in rare-earth monobismuthides with partially filled f shell. *Physical Review B*, **2018**, 98, | 3.3 | 16 |
| 58 | 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 |
| 57 | Tunable electronic structure and topological properties of LnPn (Ln=Ce, Pr, Sm, Gd, Yb; Pn=Sb, Bi). *Communications Physics*, **2018**, 1, | 5.4 | 16 |
| 56 | Reduced dimensionality and magnetic frustration in KCr3As3. *Physical Review B*, **2015**, 92, | 3.3 | 15 |
| 55 | 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 |
| 54 | From cluster to bulk: size dependent energetics of silica and silica-water interaction. *Journal of Chemical Physics*, **2006**, 124, 024722 | 3.9 | 13 |
| 53 | Unique crystal field splitting and multiband RKKY interactions in Ni-doped EuRbFe4As4. *Communications Physics*, **2019**, 2, | 5.4 | 13 |
| 52 | 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 |
| 51 | Manipulating I□V Characteristics of a Molecular Switch with Chemical Modifications. *Journal of Physical Chemistry C*, **2010**, 114, 1655-1662 | 3.8 | 12 |
| 50 | First-principles determination of the effects of intermolecular interactions on the electronic transport through molecular monolayers. *Physical Review B*, **2008**, 78, | 3.3 | 12 |
| 49 | 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 |
| 48 | Pressure induced superconductivity bordering a charge-density-wave state in NbTe with strong spin-orbit coupling. *Scientific Reports*, **2018**, 8, 6298 | 4.9 | 11 |

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| 47 | Electronic nematicity revealed by torque magnetometry in EuFe2(As1−xPx)2. *Physical Review B*, **2014**, 89, | 3.3 | 11 |
| 46 | 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 |
| 45 | Coexistence of nontrivial topological properties and strong ferromagnetic fluctuations in quasi-one-dimensional A2Cr3As3. *Npj Computational Materials*, **2020**, 6, | 10.9 | 10 |
| 44 | Large magnetoresistance and superconductivity in gallium single crystals. *Npj Quantum Materials*, **2018**, 3, | 5 | 10 |
| 43 | Lifshitz transition and nontrivial H-doping effect in the Cr-based superconductor KCr3As3Hx. *Physical Review B*, **2019**, 100, | 3.3 | 10 |
| 42 | Doping dependence of electronic structure of infinite-layer NdNiO2. *Physical Review B*, **2021**, 103, | 3.3 | 10 |
| 41 | Emerging novel electronic structure in hydrogen-Arsenene-halogen nanosheets: A computational study. *Scientific Reports*, **2017**, 7, 4773 | 4.9 | 9 |
| 40 | CaPtAs: A new noncentrosymmetric superconductor. *Science China: Physics, Mechanics and Astronomy*, **2020**, 63, 1 | 3.6 | 8 |
| 39 | Magnetic phase diagram in the Co-rich side of the LCo1−xFexAsO (L = La, Sm) system. *Physical Review B*, **2012**, 86, | 3.3 | 8 |
| 38 | First-principles simulations of dissociated and molecular H2 adsorption on Pd4-cluster-functionalized carbon nanotubes. *Physical Review B*, **2008**, 77, | 3.3 | 8 |
| 37 | Electronic structure of vacancy-ordered iron-selenide K0.5Fe1.75Se2. *Physical Review B*, **2013**, 87, | 3.3 | 7 |
| 36 | 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 |
| 35 | Predictive first-principles simulations of strain-induced phenomena at water-silica nanotube interfaces. *Journal of Chemical Physics*, **2008**, 129, 011101 | 3.9 | 7 |
| 34 | Environment dependent dynamic charge potential for silica: Application to nanoscale silica structures. *Chemical Physics Letters*, **2007**, 437, 92-98 | 2.5 | 7 |
| 33 | Quantum transport in a compensated semimetal W2As3 with nontrivial Z2 indices. *Physical Review B*, **2018**, 98, | 3.3 | 7 |
| 32 | 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 |
| 31 | Anisotropic gapping of topological Weyl rings in the charge-density-wave superconductor In TaSe2. *Science Bulletin*, **2021**, 66, 243-249 | 10.6 | 6 |
| 30 | 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 |

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| 29 | OPAL: A multiscale multicenter simulation package based on MPI-2 protocol. *International Journal of Quantum Chemistry*, **2011**, 111, 4020-4029 | 2.1 | 5 |
| 28 | 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 |
| 27 | 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 |
| 26 | Anisotropic c-f Hybridization in the Ferromagnetic Quantum Critical Metal CeRh_{6}Ge_{4}. *Physical Review Letters*, **2021**, 126, 216406 | 7.4 | 5 |
| 25 | Superconductivity in a new layered nickel selenide CsNi2Se2. *Superconductor Science and Technology*, **2016**, 29, 045008 | 3.1 | 5 |
| 24 | 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 |
| 23 | Localized 4f-electrons in the quantum critical heavy fermion ferromagnet CeRh6Ge4. *Science Bulletin*, **2021**, 66, 1389-1394 | 10.6 | 5 |
| 22 | Probing the origin of extreme magnetoresistance in Pr/Sm mono-antimonides/bismuthides. *Physical Review B*, **2019**, 99, | 3.3 | 4 |
| 21 | Enhanced anisotropic superconductivity in the topological nodal-line semimetal InxTaS2. *Physical Review B*, **2020**, 102, | 3.3 | 4 |
| 20 | Two superconducting domes separated by a possible Lifshitz transition in LaFeAs1−xPxO. *Journal of Applied Physics*, **2016**, 119, 083903 | 2.5 | 4 |
| 19 | The electronic structure of graphene tuned by hexagonal boron nitrogen layers: Semimetal–semiconductor transition. *Modern Physics Letters B*, **2016**, 30, 1650191 | 1.6 | 4 |
| 18 | Charge density wave and weak Kondo effect in a Dirac semimetal CeSbTe. *Science China: Physics, Mechanics and Astronomy*, **2021**, 64, 1 | 3.6 | 4 |
| 17 | Electron-phonon coupling and nontrivial band topology in noncentrosymmetric superconductors LaNiSi, LaPtSi, and LaPtGe. *Physical Review B*, **2020**, 101, | 3.3 | 3 |
| 16 | Kondo behavior and metamagnetic phase transition in the heavy-fermion compound CeBi2. *Physical Review B*, **2018**, 97, | 3.3 | 3 |
| 15 | Electronic structure and topological properties of centrosymmetric MoAs/WAs from first principles. *Scientific Reports*, **2017**, 7, 10491 | 4.9 | 3 |
| 14 | Prediction of spin polarized Fermi arcs in quasiparticle interference in CeBi. *Physical Review B*, **2020**, 102, | 3.3 | 3 |
| 13 | Angle-dependent magnetoresistance and its implications for Lifshitz transition in W2As3. *Npj Quantum Materials*, **2019**, 4, | 5 | 3 |
| 12 | The atomic size effect on hybrid inorganic–organic perovskite CH3NH3BI3 (B = Pb, Sn) from first-principles study. *Modern Physics Letters B*, **2017**, 31, 1750139 | 1.6 | 2 |

# List of Publications

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|---|---|---|---|
| 11 | Large magnetoresistance and large magnetothermopower effect in the Dirac material EuMnSb. *Journal of Physics Condensed Matter*, **2019**, 31, 185701 | 1.8 | 2 |
| 10 | PrBi: Topology meets quadrupolar degrees of freedom. *Physical Review B*, **2020**, 101, | 3.3 | 2 |
| 9 | Accurate projected augmented wave datasets for BaFe2As2. *New Journal of Physics*, **2010**, 12, 123029 | 2.9 | 2 |
| 8 | Coexistence of superconductivity and antiferromagentic order in Er2O2Bi with anti-ThCr2Si2 structure. *Frontiers of Physics*, **2021**, 16, 1 | 3.7 | 2 |
| 7 | Revealing the Heavy Quasiparticles in the Heavy-Fermion Superconductor CeCu_{2}Si_{2}. *Physical Review Letters*, **2021**, 127, 067002 | 7.4 | 2 |
| 6 | WannSymm: A symmetry analysis code for Wannier orbitals. *Computer Physics Communications*, **2022**, 271, 108196 | 4.2 | 1 |
| 5 | Strain-dependent optical properties of the novel monolayer group-IV dichalcogenides SiS2 semiconductor: A first-principles study. *Nanotechnology*, **2021**, | 3.4 | 1 |
| 4 | Bandwidth-control orbital-selective delocalization of 4f electrons in epitaxial Ce films. *Nature Communications*, **2021**, 12, 2520 | 17.4 | 1 |
| 3 | Cadmium and lithium doping in silver orthophosphate: An ab initio study. *Scientific Reports*, **2016**, 6, 32574 | 4.9 | 1 |
| 2 | 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 |
| 1 | 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 | |