Kailun Yao

List of Publications by Year
in descending order

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100 papers	2,599 citations	236925 25 h-index	206112 48 g-index
101 all docs	101 docs citations	101 times ranked	3252 citing authors

#	Article	IF	Citations
1	Half-metallic ferromagnetism in zinc-blendeCaC,SrC, andBaCfrom first principles. Physical Review B, 2007, 75, .	3.2	281
2	Nine New Phosphorene Polymorphs with Non-Honeycomb Structures: A Much Extended Family. Nano Letters, 2015, 15, 3557-3562.	9.1	275
3	High-efficient thermoelectric materials: The case of orthorhombic IV-VI compounds. Scientific Reports, 2015, 5, 9567.	3.3	176
4	Synthesis and Magnetic Properties of Fe3O4 Nanoparticles. Journal of Materials Synthesis and Processing, 2002, 10, 83-87.	0.3	121
5	Ferroelectricity in Covalently functionalized Two-dimensional Materials: Integration of High-mobility Semiconductors and Nonvolatile Memory. Nano Letters, 2016, 16, 7309-7315.	9.1	99
6	Synthesis of magnetite nanoparticles in W/O microemulsion. Journal of Materials Science, 2004, 39, 2633-2636.	3.7	98
7	Dirac semimetal in type-IV magnetic space groups. Physical Review B, 2018, 98, .	3.2	97
8	First-principles study of the polar (111) surface ofFe3O4. Physical Review B, 2006, 74, .	3.2	95
9	Half-metallic ferromagnetism in C-doped ZnS: Density functional calculations. Applied Physics Letters, 2009, 94, .	3.3	93
10	Engineering of charge carriersviaa two-dimensional heterostructure to enhance the thermoelectric figure of merit. Nanoscale, 2018, 10, 7077-7084.	5.6	76
11	Improved electric properties in BiFeO3 films by the doping of Ti. Journal of Sol-Gel Science and Technology, 2007, 41, 123-128.	2.4	74
12	Thermoelectric properties of half-Heusler topological insulators MPtBi (Mâ€‰=â€‰Sc, Y, La) induced by strain. Journal of Applied Physics, 2016, 119, .	2.5	46
13	Electronic structure of the organic half-metallic magnet 2-(4-nitrophenyl)-4,4,5,5-tetramethyl-4, 5-dihydro-1H-imidazol-1-oxyl 3-N-oxide. Physical Review B, 2003, 67, .	3.2	43
14	Electric properties of BiFeO3 films deposited on LaNiO3 by sol-gel process. Journal of Applied Physics, 2006, 100, 044110.	2.5	39
15	Spin transport properties based on spin gapless semiconductor CoFeMnSi. Applied Physics Letters, 2017, 111, .	3.3	37
16	Half-metallic YN₂ monolayer: dual spin filtering, dual spin diode and spin Seebeck effects. Physical Chemistry Chemical Physics, 2016, 18, 28018-28023.	2.8	35
17	The electronic and optical properties of carbon-doped SrTiO3: Density functional characterization. AIP Advances, 2012, 2, .	1.3	34
18	Half-metallic ferromagnetism in wurtzite ScM (M=C, Si, Ge, and Sn): Ab initio calculations. Applied Physics Letters, 2013, 102, .	3.3	34

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19	The peculiar transport properties in p-n junctions of doped graphene nanoribbons. Journal of Applied Physics, 2011, 110, 013718.	2.5	32
20	Two-dimensional MoS2-MoSe2 lateral superlattice with minimized lattice thermal conductivity. Journal of Applied Physics, 2018, 124, .	2.5	32
21	Nearly Perfect Spin Filter, Spin Valve and Negative Differential Resistance Effects in a Fe4-based Single-molecule Junction. Scientific Reports, 2014, 4, 4838.	3.3	31
22	First-principles study on the half-metallicity of full-Heusler alloy Co2VGa (111) surface. Journal of Applied Physics, 2012, 111, 093730.	2.5	29
23	Ultralow lattice thermal conductivity in topological insulator TlBiSe2. Applied Physics Letters, 2016, 108, .	3.3	29
24	Perfect spin filtering effect and negative differential behavior in phosphorus-doped zigzag graphene nanoribbons. Scientific Reports, 2015, 5, 15966.	3.3	28
25	Temperature-controlled colossal magnetoresistance and perfect spin Seebeck effect in hybrid graphene/boron nitride nanoribbons. Physical Chemistry Chemical Physics, 2017, 19, 4085-4092.	2.8	27
26	Electronic structure and ferromagnetism of boron doped bulk and surface CdSe: By generalized gradient approximation and generalized gradient approximation plus modified Becke and Johnson calculations. Journal of Applied Physics, 2013, 114, .	2.5	26
27	Spin transport properties of partially edge-hydrogenated MoS2 nanoribbon heterostructure. Journal of Applied Physics, 2014, 115, .	2.5	26
28	Temperature-controlled spin filter and spin valve based on Fe-doped monolayer MoS₂. Physical Chemistry Chemical Physics, 2016, 18, 6053-6058.	2.8	25
29	First-principles study of the composition, structure, and stability of the FeO (111) surface. Physical Review B, 2005, 72, .	3.2	24
30	Bulk and surface half-metallicity: Metastable zinc-blende TiSb. Journal of Applied Physics, 2012, 112, .	2.5	23
31	Large half-metallic gap in ferromagnetic semi-Heusler alloys CoCrP and CoCrAs. Applied Physics Letters, 2012, 101, 062402.	3.3	22
32	Magnetic and electronic switching properties of photochromic diarylethene with two nitronyl nitroxides. Applied Physics Letters, 2010, 97, .	3.3	21
33	Ferromagnetic properties, electronic structure, and formation energy of Ga0.9375M0.0625N (M=vacancy, Ca) by first principles study. Journal of Applied Physics, 2008, 104, 043912.	2.5	20
34	Effect of carbon/hydrogen species incorporation on electronic structure of anatase-TiO2. Journal of Applied Physics, 2011, 110, .	2.5	18
35	A new method to induce molecular low bias negative differential resistance with multi-peaks. Journal of Chemical Physics, 2016, 144, 064308.	3.0	18
36	Theoretical model of an organic ferrimagnetic state for a bipartite lozenge chain. Physical Review B, 2001, 63, .	3.2	15

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37	Surface half-metallicity in the Heusler alloy Cr2CoGa with low magnetic moment. Journal of Materials Science, 2018, 53, 8364-8371.	3.7	15
38	Ferroelectric properties and microstructures of Nd2O3-doped Bi4Ti3O12 ceramics. Physica Status Solidi A, 2003, 200, 446-450.	1.7	14
39	Controllable synthesis of large-area free-standing amorphous carbon films and their potential application in supercapacitors. RSC Advances, 2014, 4, 63734-63740.	3.6	14
40	Transfer matrix renormalization group studies on spin chains for molecule-based ferrimagnets. Physical Review B, 2004, 70, .	3.2	13
41	First-principles study of the ferromagnetic and half-metallic properties of the fumarate-bridged polymer. European Physical Journal B, 2004, 39, 283-286.	1.5	13
42	Spinâ€“lattice coupling driven ferroelectric transition in one-dimensional organic quantum magnets. Journal of Materials Chemistry, 2011, 21, 449-455.	6.7	13
43	Spin-dependent thermoelectric effects in Fe-C6 doped monolayer MoS2. Scientific Reports, 2017, 7, 497.	3.3	13
44	Rectifying behavior in La2/3Sr1/3MnO3/MgO/SrRuO3 magnetic tunnel junctions. Applied Physics Letters, 2011, 98, 172107.	3.3	12
45	Preserving stable 100% spin polarization at (111) heterostructures of half-metallic Heusler alloy Co2VGa with semiconductor PbS. Journal of Applied Physics, 2012, 112, .	2.5	12
46	The detection of HBV DNA with gold-coated iron oxide nanoparticle gene probes. Journal of Nanoparticle Research, 2008, 10, 393-400.	1.9	11
47	The half-metallic properties and geometrical structures of cubic BaMnO3 and BaTiO3/BaMnO3 superlattice. Journal of Applied Physics, 2011, 109, .	2.5	11
48	First Principles Study of Half-Metallic and Magnetic Properties of V Doped MgSiN2 Chalcopyrite. Journal of Superconductivity and Novel Magnetism, 2014, 27, 257-261.	1.8	11
49	Half-metallic ferromagnetism of chalcopyrite ZnCrAs2: A first-principles prediction. Journal of Applied Physics, 2011, 109, .	2.5	10
50	Carbon doping induced peculiar transport properties of boron nitride nanoribbons p-n junctions. Journal of Applied Physics, 2014, 116, 023708.	2.5	10
51	Boron doped GaN and InN: Potential candidates for spintronics. Journal of Applied Physics, 2017, 121, 073905.	2.5	10
52	Single-particle spectral weight of a ferromagnetic polymer chain: Cluster perturbation theory. Physical Review B, 2002, 66, .	3.2	9
53	Firstâ€principles study on the electronic structure of dilute magnetic semiconductor Ga_{1â^'x}Cr_xP in zincâ€blende phase. Physica Status Solidi (B): Basic Research, 2011, 248, 1258-1263.	1.5	9
54	The electromagnetic performance of transition metal-substituted monolayer black arsenic-phosphorus. Physical Chemistry Chemical Physics, 2021, 23, 24570-24578.	2.8	9

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55	The polaron and bipolaron states of poly(phenylene vinylene). Journal of Chemical Physics, 2001, 114, 6437-6442.	3.0	8
56	Ab initiostudy of the spin distribution and conductive properties of a Malonato-bridged gadolinium (III) complex. Physical Review B, 2007, 76, .	3.2	8
57	Efficient spin-filter and negative differential resistance behaviors in FeN4 embedded graphene nanoribbon device. Journal of Applied Physics, 2016, 119, .	2.5	8
58	Multiple thermal spin transport performances of graphene nanoribbon heterojuction co-doped with Nitrogen and Boron. Scientific Reports, 2017, 7, 3955.	3.3	8
59	First-Principles Study on the Thermoelectric Properties of FeAsS. ACS Omega, 2018, 3, 13630-13635.	3.5	8
60	Potential outstanding physical properties of novel black arsenic phosphorus As_{0.25}P_{0.75}/As_{0.75}P_{0.25} phases: a first-principles investigation. RSC Advances, 2022, 12, 3745-3754.	3.6	8
61	Polaronic excitations in the doped polyacene. Zeitschrift FÃ¼r Physik B-Condensed Matter, 1997, 104, 77-80.	1.1	7
62	Preparation and characterization of micron-sized magnetic microspheres by one-step suspension polymerization. Journal of Applied Polymer Science, 2007, 105, 1331-1335.	2.6	7
63	LOCALIZATION OF THE ENERGY STATES OF LEAD INDUCING THE EFFECT OF RECTIFICATION AND NEGATIVE DIFFERENTIAL RESISTANCE PREDICTED BY FIRST-PRINCIPLES STUDY. International Journal of Modern Physics B, 2013, 27, 1350081.	2.0	7
64	First-principles study of doping-induced half-metallicity at the (001) surface of full-Heusler alloy Co2VGa. Journal of Applied Physics, 2013, 114, 143712.	2.5	7
65	Contact transparency inducing low bias negative differential resistance in two capped carbon nanotubes sandwiching Ïƒ barrier. Applied Physics A: Materials Science and Processing, 2015, 118, 367-371.	2.3	7
66	Anomalous temperature effect of nonlinearity of WO3 varistor doped with Al2O3. Science Bulletin, 1999, 44, 671-672.	1.7	6
67	Temperature characteristics of electrical behavior of W-Bi-Ti-O ceramics at low field. Science Bulletin, 2004, 49, 313-316.	1.7	6
68	Half-metallicity and tetragonal distortion in semi-Heusler alloy FeCrSe. Journal of Applied Physics, 2014, 115, 043713.	2.5	6
69	Tuning of the electronic structures and spin-dependent transport properties of phosphorene nanoribbons by vanadium substitutional doping. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 138, 115067.	2.7	6
70	Dual spin filtering and negative differential resistance effects in vanadium doped zigzag phosphorene nanoribbons with different edge passivations. AIP Advances, 2022, 12, .	1.3	6
71	Electrical Properties of Nanocrystalline CeO2â€“Y2O3 Thin Films Prepared by the Sol-Gel Method. Inorganic Materials, 2003, 39, 720-724.	0.8	5
72	Morphological evolution of Nb2O5 in a solvothermal reaction: From Nb2O5 grains to Nb2O5 nanorods and hexagonal Nb2O5 nanoplatelets. Journal Wuhan University of Technology, Materials Science Edition, 2009, 24, 245-248.	1.0	5

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73	Magnetic-field-driven quantum criticality and thermodynamics in trimerized spin-1/2 isotropic XY chain with three-spin interactions. Physica Status Solidi (B): Basic Research, 2010, 247, 2274-2283.	1.5	5
74	A theoretical model for anisotropic multiferroics. Applied Physics Letters, 2013, 103, 132911.	3.3	5
75	Bulk and surface half-metallicity: The case of D03-type Mn3Ge. Journal of Applied Physics, 2014, 115, 033704.	2.5	5
76	A First Principles Study of the Electronic Structures and Tetragonal Distortion of the Ti2NiGa Heusler Alloy. Journal of Superconductivity and Novel Magnetism, 2014, 27, 1579-1585.	1.8	5
77	Nearly Perfect Spin Filter Based on a Wire of Half-Metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo		

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91	Efficient spin-filtering, magnetoresistance and negative differential resistance effects of a one-dimensional single-molecule magnet Mn(dmit)2-based device with graphene nanoribbon electrodes. AIP Advances, 2017, 7, .	1.3	2
92	Effects of Electron-Electron Interactions on the Ferromagnetic State in an Organic Polaronic Ferromagnet. Physica Status Solidi (B): Basic Research, 1998, 209, 173-178.	1.5	0
93	Interchain Coupling and Electronic Band Structure in Polydiacetylenes. Molecular Crystals and Liquid Crystals, 1999, 337, 341-344.	0.3	0
94	DMRG studies on interchain coupling model for quasi-one-dimensional organic magnet. European Physical Journal B, 2003, 35, 365-370.	1.5	0
95	Spin and lattice configurationsin p-conjugated organic ferromagnetic polymerwith open boundary condition. Physica Status Solidi (B): Basic Research, 2003, 239, 426-431.	1.5	0
96	The electronic structure and the ferromagnetic intermolecular interactions in the crystal of a diphenyl nitroxide derivative. Philosophical Magazine, 2007, 87, 4119-4129.	1.6	0
97	The effect of state disproportion on Na0.5CoO2 and other NaxCoO2 compounds. Journal of Applied Physics, 2010, 107, 083710.	2.5	0
98	Magnetic property of a spin-5/2 trigonal prismatic as a model for a molecule-based compound Cs4Na7[Fe6(OH)3(A-Î±-GeW9O34(OH)3)2]ãƒ»30H2O. Journal Wuhan University of Technology, Materials Science Edition, 2015, 30, 868-872.	1.0	0
99	Large magnetoelectric effect in the strained CoPt/SrTiO3 junction. Journal of Applied Physics, 2017, 122, 065302.	2.5	0
100	Negative differential resistance and spin filter effects in VS2 monolayers. RSC Advances, 2017, 7, 33733-33736.	3.6	0