

Kailun Yao

List of Publications by Year in descending order

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100
papers

2,599
citations

236925

25
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206112

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101
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101
docs citations

101
times ranked

3252
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning of the electronic structures and spin-dependent transport properties of phosphorene nanoribbons by vanadium substitutional doping. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 138, 115067.	2.7	6
2	Dual spin filtering and negative differential resistance effects in vanadium doped zigzag phosphorene nanoribbons with different edge passivations. <i>AIP Advances</i> , 2022, 12, .	1.3	6
3	Potential outstanding physical properties of novel black arsenic phosphorus $\text{As}_{0.25}\text{P}_{0.75}/\text{As}_{0.75}\text{P}_{0.25}$ phases: a first-principles investigation. <i>RSC Advances</i> , 2022, 12, 3745-3754.	3.6	8
4	Spin-polarized transport properties of the $\text{FeCl}_2/\text{WSe}_2/\text{FeCl}_2$ van der Waals heterostructure. <i>Applied Physics Letters</i> , 2022, 120, .	3.3	3
5	The electromagnetic performance of transition metal-substituted monolayer black arsenic-phosphorus. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24570-24578.	2.8	9
6	<i>Ab initio</i> calculation of transport properties in 1,3-diphenylpropynylidene based molecular device. <i>Molecular Physics</i> , 2020, 118, .	1.7	3
7	Surface half-metallicity in the Heusler alloy Cr_2CoGa with low magnetic moment. <i>Journal of Materials Science</i> , 2018, 53, 8364-8371.	3.7	15
8	Engineering of charge carriers via a two-dimensional heterostructure to enhance the thermoelectric figure of merit. <i>Nanoscale</i> , 2018, 10, 7077-7084.	5.6	76
9	Dirac semimetal in type-IV magnetic space groups. <i>Physical Review B</i> , 2018, 98, .	3.2	97
10	First-Principles Study on the Thermoelectric Properties of FeAsS . <i>ACS Omega</i> , 2018, 3, 13630-13635.	3.5	8
11	Two-dimensional MoS_2 - MoSe_2 lateral superlattice with minimized lattice thermal conductivity. <i>Journal of Applied Physics</i> , 2018, 124, .	2.5	32
12	Temperature-controlled colossal magnetoresistance and perfect spin Seebeck effect in hybrid graphene/boron nitride nanoribbons. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4085-4092.	2.8	27
13	Boron doped GaN and InN: Potential candidates for spintronics. <i>Journal of Applied Physics</i> , 2017, 121, 073905.	2.5	10
14	Spin-dependent thermoelectric effects in Fe-C6 doped monolayer MoS_2 . <i>Scientific Reports</i> , 2017, 7, 497.	3.3	13
15	Spin transport properties based on spin gapless semiconductor CoFeMnSi . <i>Applied Physics Letters</i> , 2017, 111, .	3.3	37
16	Large magnetoelectric effect in the strained $\text{CoPt}/\text{SrTiO}_3$ junction. <i>Journal of Applied Physics</i> , 2017, 122, 065302.	2.5	0
17	Negative differential resistance and spin filter effects in VS_2 monolayers. <i>RSC Advances</i> , 2017, 7, 33733-33736.	3.6	0
18	Multiple thermal spin transport performances of graphene nanoribbon heterojunction co-doped with Nitrogen and Boron. <i>Scientific Reports</i> , 2017, 7, 3955.	3.3	8

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19	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
20	A new method to induce molecular low bias negative differential resistance with multi-peaks. Journal of Chemical Physics, 2016, 144, 064308.	3.0	18
21	Efficient spin-filter and negative differential resistance behaviors in FeN ₄ embedded graphene nanoribbon device. Journal of Applied Physics, 2016, 119, .	2.5	8
22	Ultralow lattice thermal conductivity in topological insulator TlBiSe ₂ . Applied Physics Letters, 2016, 108, .	3.3	29
23	Thermoelectric properties of half-Heusler topological insulators MPtBi (M = Sc, Y, La) induced by strain. Journal of Applied Physics, 2016, 119, .	2.5	46
24	Half-metallic YN ₂ monolayer: dual spin filtering, dual spin diode and spin Seebeck effects. Physical Chemistry Chemical Physics, 2016, 18, 28018-28023.	2.8	35
25	Ferroelectricity in Covalently functionalized Two-dimensional Materials: Integration of High-mobility Semiconductors and Nonvolatile Memory. Nano Letters, 2016, 16, 7309-7315.	9.1	99
26	Temperature-controlled spin filter and spin valve based on Fe-doped monolayer MoS ₂ . Physical Chemistry Chemical Physics, 2016, 18, 6053-6058.	2.8	25
27	Prediction of large magnetoelectric coupling in Fe ₄ N/BaTiO ₃ and MnFe ₃ N/BaTiO ₃ junctions from a first-principles study. RSC Advances, 2016, 6, 29504-29511. Nearly Perfect Spin Filter Based on a Wire of Half-Metallic	3.6	5
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37	Spin transport properties of partially edge-hydrogenated MoS ₂ nanoribbon heterostructure. Journal of Applied Physics, 2014, 115, .	2.5	26
38	First Principles Study of Half-Metallic and Magnetic Properties of V Doped MgSiN ₂ Chalcopyrite. Journal of Superconductivity and Novel Magnetism, 2014, 27, 257-261.	1.8	11
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	A First Principles Study of the Electronic Structures and Tetragonal Distortion of the Ti ₂ NiGa Heusler Alloy. Journal of Superconductivity and Novel Magnetism, 2014, 27, 1579-1585.	1.8	5
41	Nearly Perfect Spin Filter, Spin Valve and Negative Differential Resistance Effects in a Fe ₄ -based Single-molecule Junction. Scientific Reports, 2014, 4, 4838.	3.3	31
42	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
43	A theoretical model for anisotropic multiferroics. Applied Physics Letters, 2013, 103, 132911.	3.3	5
44	Half-metallic ferromagnetism in wurtzite ScM (M=C, Si, Ge, and Sn): Ab initio calculations. Applied Physics Letters, 2013, 102, .	3.3	34
45	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
46	First-principles study of doping-induced half-metallicity at the (001) surface of full-Heusler alloy Co ₂ VGa. Journal of Applied Physics, 2013, 114, 143712.	2.5	7
47	First-principles study on the half-metallicity of full-Heusler alloy Co ₂ VGa (111) surface. Journal of Applied Physics, 2012, 111, 093730.	2.5	29
48	Large half-metallic gap in ferromagnetic semi-Heusler alloys CoCrP and CoCrAs. Applied Physics Letters, 2012, 101, 062402.	3.3	22
49	Preserving stable 100% spin polarization at (111) heterostructures of half-metallic Heusler alloy Co ₂ VGa with semiconductor PbS. Journal of Applied Physics, 2012, 112, .	2.5	12
50	Bulk and surface half-metallicity: Metastable zinc-blende TiSb. Journal of Applied Physics, 2012, 112, .	2.5	23
51	Anisotropic transport properties of zinc-blend ZnTe/CrTe heterogeneous junction nanodevices. Journal of Applied Physics, 2012, 112, .	2.5	3
52	The electronic and optical properties of carbon-doped SrTiO ₃ : Density functional characterization. AIP Advances, 2012, 2, .	1.3	34
53	Half metallicity through wide range of lattice constants in Heusler alloys Co ₂ MnGa _{1-x} Ge _x : First-principles calculations. Physica Status Solidi (B): Basic Research, 2012, 249, 840-846.	1.5	2
54	Spin-lattice coupling driven ferroelectric transition in one-dimensional organic quantum magnets. Journal of Materials Chemistry, 2011, 21, 449-455.	6.7	13

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55	Rectifying behavior in La ₂ /3Sr ₁ /3MnO ₃ /MgO/SrRuO ₃ magnetic tunnel junctions. Applied Physics Letters, 2011, 98, 172107.	3.3	12
56	Half-metallic ferromagnetism of chalcopyrite ZnCrAs ₂ : A first-principles prediction. Journal of Applied Physics, 2011, 109, .	2.5	10
57	Electronic structure and half-metallic property of Si ₃ CaC ₄ . European Physical Journal B, 2011, 83, 319-323.	1.5	4
58	First-principles study on the electronic structure of dilute magnetic semiconductor Ga _{1-x} Cr _x P in zinc-blende phase. Physica Status Solidi (B): Basic Research, 2011, 248, 1258-1263.	1.5	9
59	The half-metallic properties and geometrical structures of cubic BaMnO ₃ and BaTiO ₃ /BaMnO ₃ superlattice. Journal of Applied Physics, 2011, 109, .	2.5	11
60	Effect of carbon/hydrogen species incorporation on electronic structure of anatase-TiO ₂ . Journal of Applied Physics, 2011, 110, .	2.5	18
61	Ab initio investigation of the noncollinear magnetic structure of CeFeAsO. Physical Review B, 2011, 84, .	3.2	2
62	The peculiar transport properties in p-n junctions of doped graphene nanoribbons. Journal of Applied Physics, 2011, 110, 013718.	2.5	32
63	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
64	The effect of state disproportionation on Na _{0.5} CoO ₂ and other Na _x CoO ₂ compounds. Journal of Applied Physics, 2010, 107, 083710.	2.5	0
65	Magnetic and electronic switching properties of photochromic diarylethene with two nitronyl nitroxides. Applied Physics Letters, 2010, 97, .	3.3	21
66	Morphological evolution of Nb ₂ O ₅ in a solvothermal reaction: From Nb ₂ O ₅ grains to Nb ₂ O ₅ nanorods and hexagonal Nb ₂ O ₅ nanoplatelets. Journal Wuhan University of Technology, Materials Science Edition, 2009, 24, 245-248.	1.0	5
67	Half-metallic ferromagnetism in C-doped ZnS: Density functional calculations. Applied Physics Letters, 2009, 94, .	3.3	93
68	The detection of HBV DNA with gold-coated iron oxide nanoparticle gene probes. Journal of Nanoparticle Research, 2008, 10, 393-400.	1.9	11
69	Ferromagnetic properties, electronic structure, and formation energy of Ga _{0.9375} M _{0.0625} N (M=vacancy, Ca) by first principles study. Journal of Applied Physics, 2008, 104, 043912.	2.5	20
70	Atomic, electronic, and magnetic structure of the Au(100)•Fe ₃ O ₄ (100) interface: Density functional theory study. Physical Review B, 2007, 75, .	3.2	4
71	Ab initio study of the spin distribution and conductive properties of a Malonato-bridged gadolinium (III) complex. Physical Review B, 2007, 76, .	3.2	8
72	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

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73	Half-metallic ferromagnetism in zinc-blende CaC , SrC , and BaC from first principles. <i>Physical Review B</i> , 2007, 75, .	3.2	281
74	Preparation and characterization of micron-sized magnetic microspheres by one-step suspension polymerization. <i>Journal of Applied Polymer Science</i> , 2007, 105, 1331-1335.	2.6	7
75	Improved electric properties in BiFeO_3 films by the doping of Ti. <i>Journal of Sol-Gel Science and Technology</i> , 2007, 41, 123-128.	2.4	74
76	Characterization and application of magnetic P (St-co-MAA-co-AM)/ SiO_2 composite microspheres. <i>Journal of Materials Science</i> , 2007, 42, 5147-5151.	3.7	3
77	Electric properties of BiFeO_3 films deposited on LaNiO_3 by sol-gel process. <i>Journal of Applied Physics</i> , 2006, 100, 044110.	2.5	39
78	First-principles study of the polar (111) surface of Fe_3O_4 . <i>Physical Review B</i> , 2006, 74, .	3.2	95
79	Electrical properties of undoped PZT and Co-doped PCZT films deposited on ITO/glass substrates by a sol-gel method. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2005, 202, 1834-1841.	1.8	3
80	First-principles study of the composition, structure, and stability of the FeO (111) surface. <i>Physical Review B</i> , 2005, 72, .	3.2	24
81	Transfer matrix renormalization group studies on spin chains for molecule-based ferrimagnets. <i>Physical Review B</i> , 2004, 70, .	3.2	13
82	First-principles study of the ferromagnetic and half-metallic properties of the fumarate-bridged polymer. <i>European Physical Journal B</i> , 2004, 39, 283-286.	1.5	13
83	Synthesis of magnetite nanoparticles in W/O microemulsion. <i>Journal of Materials Science</i> , 2004, 39, 2633-2636.	3.7	98
84	Temperature characteristics of electrical behavior of W-Bi-Ti-O ceramics at low field. <i>Science Bulletin</i> , 2004, 49, 313-316.	1.7	6
85	DMRG studies on interchain coupling model for quasi-one-dimensional organic magnet. <i>European Physical Journal B</i> , 2003, 35, 365-370.	1.5	0
86	Electrical Properties of Nanocrystalline CeO_2 - Y_2O_3 Thin Films Prepared by the Sol-Gel Method. <i>Inorganic Materials</i> , 2003, 39, 720-724.	0.8	5
87	Ferroelectric properties and microstructures of Nd_2O_3 -doped $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ ceramics. <i>Physica Status Solidi A</i> , 2003, 200, 446-450.	1.7	14
88	Spin and lattice configurations in p-conjugated organic ferromagnetic polymer with open boundary condition. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 239, 426-431.	1.5	0
89	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. <i>Physical Review B</i> , 2003, 67, .	3.2	43
90	Single-particle spectral weight of a ferromagnetic polymer chain: Cluster perturbation theory. <i>Physical Review B</i> , 2002, 66, .	3.2	9

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91	Synthesis and Magnetic Properties of Fe ₃ O ₄ Nanoparticles. Journal of Materials Synthesis and Processing, 2002, 10, 83-87.	0.3	121
92	The polaron and bipolaron states of poly(phenylene vinylene). Journal of Chemical Physics, 2001, 114, 6437-6442.	3.0	8
93	Theoretical model of an organic ferrimagnetic state for a bipartite lozenge chain. Physical Review B, 2001, 63, .	3.2	15
94	Effects of electron-electron interaction on the band structure in polydiacetylenes. Journal of Polymer Science, Part B: Polymer Physics, 2000, 38, 1656-1661.	2.1	3
95	Anomalous temperature effect of nonlinearity of WO ₃ varistor doped with Al ₂ O ₃ . Science Bulletin, 1999, 44, 671-672.	1.7	6
96	Interchain Coupling and Electronic Band Structure in Polydiacetylenes. Molecular Crystals and Liquid Crystals, 1999, 337, 341-344.	0.3	0
97	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
98	Overview on grain-boundary and transport problems in solid oxide fuel cell. Ionics, 1998, 4, 472-476.	2.4	4
99	Stability and Spin Density in Doped Quasi-One-Dimensional Non-Conjugated Organic Ferromagnets. Modern Physics Letters B, 1998, 12, 1125-1132.	1.9	2
100	Polaronic excitations in the doped polyacene. Zeitschrift für Physik B-Condensed Matter, 1997, 104, 77-80.	1.1	7