

Jaejun Yu

List of Publications by Year in descending order

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7497
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#	ARTICLE	IF	CITATIONS
1	Band gap narrowing of TiO ₂ nanoparticles: A passivated Co-doping approach for enhanced photocatalytic activity. Journal of Physics and Chemistry of Solids, 2022, 162, 110503.	4.0	9
2	Structure and disorder in MgSiO ₃ glasses above megabar pressures via nuclear magnetic resonance: DFT calculations. Journal of the American Ceramic Society, 2022, 105, 5151-5166.	3.8	3
3	Chirality-induced spin texture switching in twisted bilayer graphene. Physical Review B, 2021, 104, .	3.2	5
4	Inevitable high density of oxygen vacancies at the surface of polar/nonpolar perovskite heterostructures LaAlO ₃ /SrTiO ₃ . Journal of Applied Physics, 2020, 127, .	2.5	6
5	Chern insulator with a nearly flat band in the metal-organic-framework-based Kagome lattice. Scientific Reports, 2019, 9, 13807.	3.3	17
6	Multiferroic Materials: A Room-Temperature Ferroelectric Ferromagnet in a 1D Tetrahedral Chain Network (Adv. Mater. 24/2019). Advanced Materials, 2019, 31, 1970173.	21.0	3
7	A Room-Temperature Ferroelectric Ferromagnet in a 1D Tetrahedral Chain Network. Advanced Materials, 2019, 31, e1808104.	21.0	22
8	Superstructures of Se adsorbates on Au(111): Scanning tunneling microscopy and spectroscopy study. Surface Science, 2019, 685, 19-23.	1.9	4
9	Effect of Coulomb Interactions on the Electronic and Magnetic Properties of Two-Dimensional CrSiTe ₃ and CrGeTe ₃ Materials. Journal of Electronic Materials, 2019, 48, 1441-1445.	2.2	34
10	Graphene analogue in (111)-oriented BaBiO ₃ bilayer heterostructures for topological electronics. Scientific Reports, 2018, 8, 555.	3.3	6
11	Half-metallic ferromagnetism and metal-insulator transition in Sn-doped SrRuO ₃ perovskite oxides. Journal of Magnetism and Magnetic Materials, 2018, 460, 54-60.	2.3	13
12	Magnetic states and intervalence charge transfer of Ti and Fe defects in γ -Al ₂ O ₃ : The origin of the blue in sapphire. Acta Materialia, 2018, 143, 248-256.	7.9	10
13	Identification of F impurities in F-doped ZnO by synchrotron X-ray absorption near edge structures. Journal of Applied Physics, 2018, 123, 161528.	2.5	1
14	Tunable magnetic topological insulating phases in monolayer CrI ₃ . Physical Review B, 2018, 98, .	3.2	33
15	Role of oxygen vacancy in the spin-state change and magnetic ordering in SrCoO _{3-x} . Physical Review B, 2018, 98, .	3.2	33
16	Magnetic interactions in PdCrO ₂ and their effects on its magnetic structure. Physical Review B, 2018, 98, .	3.2	33
17	Band gap and mobility of epitaxial perovskite BaSn _{1-x} Hf _x O ₃ thin films. Physical Review Materials, 2018, 2, .	2.4	3
18	Passivated co-doping approach to bandgap narrowing of titanium dioxide with enhanced photocatalytic activity. Applied Catalysis B: Environmental, 2017, 200, 1-9.	20.2	90

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19	High-k perovskite gate oxide BaHfO ₃ . APL Materials, 2017, 5, .	5.1	28
20	<i>Ab Initio</i> Study of Elastic Properties of High-Pressure Polymorphs of CO ₂ Phases II and V. Journal of Physical Chemistry C, 2016, 120, 23152-23164.	3.1	7
21	All-perovskite transparent high mobility field effect using epitaxial BaSnO ₃ and LaInO ₃ . APL Materials, 2015, 3, .	5.1	107
22	Impact of vacancy clusters on characteristic resistance change of nonstoichiometric strontium titanate nano-film. Applied Physics Letters, 2014, 104, .	3.3	15
23	Dopant-site-dependent scattering by dislocations in epitaxial films of perovskite semiconductor BaSnO ₃ . APL Materials, 2014, 2, .	5.1	61
24	Charge and magnetic states of rutile TiO ₂ doped with Cr ions. Journal of Physics Condensed Matter, 2014, 26, 146003.	1.8	10
25	Strain-induced topological insulator phase and effective magnetic interactions in Li ₂ IrO ₃ . Physical Review B, 2013, 87, .	3.2	35
26	Large in-plane deformation of RuO ₆ octahedron and ferromagnetism of bulk SrRuO ₃ . Journal of Physics Condensed Matter, 2013, 25, 465601.	1.8	23
27	Enhanced upper critical fields in a new quasi-one-dimensional superconductor Nb ₂ Pd _x Se ₅ . New Journal of Physics, 2013, 15, 123031.	2.9	35
28	Collinear and noncollinear spin ground state of wurtzite CoO. Physical Review B, 2013, 87, .	3.2	10
29	Indications of strong neutral impurity scattering in Ba(Sn,Sb)O ₃ single crystals. Physical Review B, 2013, 88, .	3.2	48
30	Two-dimensional electron gas generated by La-doping at SrTiO ₃ (001) surface: A first-principles study. AIP Advances, 2013, 3, 062116.	1.3	2
31	Modulation of electron carrier density at the n-type LaAlO ₃ /SrTiO ₃ interface by water adsorption. Journal of Physics Condensed Matter, 2013, 25, 265004.	1.8	11
32	Effective Control of the Charge and Magnetic States of Transition-Metal Atoms on Single-Layer Boron Nitride. Physical Review Letters, 2012, 108, 206802.	7.8	135
33	Spin and orbital angular momentum structure of Cu(111) and Au(111) surface states. Physical Review B, 2012, 85, .	3.2	67
34	Physical properties of transparent perovskite oxides (Ba,La)SnO ₃ with high electrical mobility at room temperature. Physical Review B, 2012, 86, Transition in	3.2	264
35	Transition Metal Oxide Na ₂ IrO ₂ . Physical Review Letters, 2012, 108, 106401	7.8	87
36	Orbital-Angular-Momentum Based Origin of Rashba-Type Surface Band Splitting. Physical Review Letters, 2011, 107, 156803.	7.8	162

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37	Effect of oxygen vacancies and charge carriers induced in the n -type interface of a LaAlO ₃ overlayer on SrTiO ₃ . <i>Chemical Physics Letters</i> , 2010, 492, 89-92.	3.2	99
38	Effect of on-site Coulomb interactions on the electronic structure and magnetic property of Gd ₂ cluster. <i>Chemical Physics Letters</i> , 2010, 492, 89-92.	2.6	4
39	Polarization screening and induced carrier density at the interface of LaAlO ₃ overlayer on SrTiO ₃ (001). <i>Journal of Applied Physics</i> , 2010, 108, .	2.5	17
40	Tunable charge donation and spin polarization of metal adsorbates on graphene using an applied electric field. <i>Physical Review B</i> , 2010, 82, .	3.2	13
41	First-principles study of ultrathin (2 \bar{A} -2) Gd nanowires encapsulated in carbon nanotubes. <i>Journal of Chemical Physics</i> , 2010, 132, 054701.	3.0	19
42	Mapping Atomic Contact between Pentacene and a Au Surface using Scanning Tunneling Spectroscopy. <i>Nano Letters</i> , 2010, 10, 996-999.	9.1	13
43	Possible origins of defect-induced magnetic ordering in carbon-irradiated graphite. <i>Physical Review B</i> , 2009, 79, .	3.2	15
44	Origin of reduced polarizations in short-period BaTiO ₃ /SrTiO ₃ ferroelectric superlattices. <i>Journal of Applied Physics</i> , 2009, 105, .	2.5	17
45	Competition between structural distortion and magnetic moment formation in fullerene C ₂₀ . <i>Journal of Chemical Physics</i> , 2009, 130, 184107.	3.0	12
46	Structure and magnetism of small Gd and Fe nanoclusters: LDA calculations. <i>Solid State Communications</i> , 2009, 149, 2058-2060.	1.9	14
47	Anisotropic exchange interactions of spin-orbit-integrated states in Sr ₂ IrO ₇ . <i>Physical Review Letters</i> , 2009, 103, 077202.	3.2	117
48	Novel π - π interaction induced by relativistic spin-orbit coupling in Sr_2IrO_7 . <i>Physical Review Letters</i> , 2008, 101, 076402.	7.8	1,332
49	Electronic structures of hexagonal RMnO ₃ (R=Gd, Tb, Dy, and Ho) thin films: Optical spectroscopy and first-principles calculations. <i>Physical Review B</i> , 2008, 77, .	3.2	75
50	Photonic crystal alloys: a new twist in controlling photonic band structure properties. <i>Optics Express</i> , 2008, 16, 6579.	3.4	7
51	Doped valence-bond solid and superconductivity on the Shastry-Sutherland lattice. <i>Physical Review B</i> , 2008, 77, .	3.2	10
52	Interaction and ordering of vacancy defects in NiO. <i>Physical Review B</i> , 2008, 77, .	3.2	118
53	Spin triplet excitations for a valence bond solid on the kagome lattice. <i>Physical Review B</i> , 2008, 77, .	3.2	23
54	First-principles effective Hamiltonian for ferroelectric polarization in BaTiO ₃ /SrTiO ₃ superlattices. <i>Journal of Applied Physics</i> , 2008, 103, 124106.	2.5	15

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55	Electronic Structure and Insulating Nature of the (LaTiO ₃) ₂ /(LaAlO ₃) ₂ Superlattice. Journal of the Korean Physical Society, 2008, 53, 1074-1078.	0.7	3
56	A spin-dependent local moment approach to the Anderson impurity model. Journal of Physics Condensed Matter, 2007, 19, 456203.	1.8	2
57	Interface electronic structure, two-dimensional metallicity, and possible interface superconductivity in CuCl_2/Si superlattices. Physical Review B, 2007, 76, .	3.2	6
58	Comparison of localized basis and plane-wave basis for density-functional calculations of organic molecules on metals. Physical Review B, 2007, 75, .	3.2	64
59	Formation of carbon nanotube semiconductor-metal intramolecular junctions by self-assembly of vacancy defects. Physical Review B, 2007, 76, .	3.2	32
60	Enhanced Charge Gap in the Bilayer Manganite $\text{La}_{2-x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ near $x=0.4$. Physical Review Letters, 2007, 98, 187201.	7.8	11
61	Magnetic ordering and exchange interactions in multiferroic GaFeO_3 . Physical Review B, 2007, 75, .	3.2	74
62	Synthesis, Characterization, and Self-Assembly of Pencil-Shaped CoO Nanorods. Journal of the American Chemical Society, 2006, 128, 9753-9760.	13.7	201
63	Effect of Orbital Rotation and Mixing on the Optical Properties of Orthorhombic RMnO_3 (R=La, Pr, Nd). $T_j \text{ ETQq1 } 10, 784314 \text{ rgBT / Ov}$	7.8	45
64	O(N)LDA+U electronic structure calculation method based on the nonorthogonal pseudoatomic orbital basis. Physical Review B, 2006, 73, .	3.2	118
65	Missing γ -Band Fermi Surface in 4d Transition-Metal Oxide Sr_2RhO_4 : Effect of the Octahedra Rotation on the Electronic Structure. Physical Review Letters, 2006, 97, 106401.	7.8	50
66	Ab initio study of pentacene on Au(001) surface. Surface Science, 2005, 589, 8-18.	1.9	54
67	Band gap sensitivity of bromine adsorption at carbon nanotubes. Chemical Physics Letters, 2005, 403, 135-139.	2.6	30
68	Current Status of Women Physicists in Korea. AIP Conference Proceedings, 2005, , .	0.4	0
69	Magnetic ordering at the edges of graphitic fragments: Magnetic tail interactions between the edge-localized states. Physical Review B, 2005, 72, .	3.2	487
70	Ferromagnetism at the edges of the stacked graphitic fragments: an ab initio study. Chemical Physics Letters, 2004, 398, 207-211.	2.6	36
71	Electronic structure, magnetic interactions, and the role of ligands in $\text{Mn}^{n=4,12}$ single-molecule magnets. Physical Review B, 2004, 70, .	3.2	58
72	Heat-Induced Transformation of Nanodiamond into a Tube-Shaped Fullerene: A Molecular Dynamics Simulation. Physical Review Letters, 2003, 91, 265701.	7.8	45

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73	Electron and Orbital Correlations in $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ Probed by Optical Spectroscopy. <i>Physical Review Letters</i> , 2002, 89, 257402.	7.8	77
74	Energetics of large carbon clusters: Crossover from fullerenes to nanotubes. <i>Physical Review B</i> , 2002, 65, .	3.2	32
75	Catalytic decomposition of acetylene on Fe(001): A first-principles study. <i>Physical Review B</i> , 2002, 66, .	3.2	22
76	Optical properties of BaRuO_3 : observation of pseudogap formation. <i>Current Applied Physics</i> , 2001, 1, 163-167.	2.4	2
77	Pseudogap formation in 4 d transition metal oxide BaRuO_3 . <i>Europhysics Letters</i> , 2001, 55, 280-286.	2.0	48
78	Suppression of ferromagnetic ordering in doped manganites: Effects of the superexchange interaction. <i>Physical Review B</i> , 2000, 61, 428-431.	3.2	14
79	Optical investigations of the charge gap in orbital-ordered $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$. <i>Physical Review B</i> , 2000, 61, 6902-6906.	3.2	30
80	Dimensional crossover driven by magnetic ordering in optical conductivity of $\text{Pr}_{1/2}\text{Sr}_{1/2}\text{MnO}_3$. <i>Physical Review B</i> , 2000, 61, 14656-14659.	3.2	11
81	Long-range hopping correlation and colossal magnetoresistance in doped manganites. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 5453-5462.	1.8	3
82	Anomalous spin susceptibility and magnetic polaron formation in the double-exchange systems. <i>Physical Review B</i> , 2000, 61, 9501-9505.	3.2	34
83	Midgap states of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$: Doping-dependent optical-conductivity studies. <i>Physical Review B</i> , 1998, 57, R11043-R11046.	3.2	98
84	Scaling Behavior of Spectral Weight Changes in Perovskite Manganites $\text{La}_{0.7-x}\text{Pr}_x\text{Ca}_{0.3}\text{MnO}_3$. <i>Physical Review Letters</i> , 1998, 81, 4983-4986.	7.8	35
85	Double-exchange model with background superexchange interactions: Phase diagrams of $\text{La}_{1-x}\text{A}_x\text{MnO}_3$ manganites. <i>Physical Review B</i> , 1998, 58, 11123-11126.	3.2	21
86	Induced vortex dynamics in parallel Josephson junction arrays. <i>Physical Review B</i> , 1997, 55, 1231-1235.	3.2	6
87	Determination of electronic band structures of CaMnO_3 and LaMnO_3 using optical-conductivity analyses. <i>Physical Review B</i> , 1997, 55, 15489-15493.	3.2	134
88	Dynamical properties of high-temperature-superconductor granular bridge junctions: Inhomogeneous Josephson-junction-array model. <i>Physical Review B</i> , 1996, 53, 3578-3584.	3.2	3
89	Pressure-induced phonon softening and electronic topological transition in $\text{HgBa}_2\text{CuO}_4$. <i>Physical Review B</i> , 1996, 54, 1313-1319.	3.2	21
90	Current-voltage characteristics and Josephson ac effects of granular HTSC $\text{YBa}_2\text{Cu}_3\text{O}_y$ bridges. <i>Solid State Communications</i> , 1995, 94, 45-48.	1.9	0

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91	Micro-Raman study of the role of pressure in mercury-based superconductors. Physical Review B, 1995, 51, 644-647.	3.2	16
92	Raman modes of the apical oxygen in mercury-based superconductors. Physical Review B, 1995, 52, 15078-15081.	3.2	17
93	Orientations of oxygen hole states and ionicity of bismuth atoms in Bi ₂ Sr ₂ CaCu ₂ O ₈ . Physical Review B, 1994, 50, 6370-6374.	3.2	17
94	Electronic band structure of high T _c Cu-oxide superconductors: Comparison of predictions with experiments. Journal of Electron Spectroscopy and Related Phenomena, 1994, 66, 281-301.	1.7	7
95	Electronic structure and properties of vacancy-ordered YBa ₂ Cu ₃ O _{6.5} . Physica C: Superconductivity and Its Applications, 1993, 214, 335-344.	1.2	11
96	Hole states in CuO ₂ planes and Cu-O chains of YBa ₂ Cu ₃ O ₇ and YBa ₂ Cu ₄ O ₈ probed by soft-x-ray absorption spectroscopy. Physical Review B, 1992, 45, 2581-2584.	3.2	54
97	Two-photon momentum density in La _{2-x} Sr _x CuO ₄ and Nd _{2-x} Ce _x CuO ₄ . Physical Review B, 1992, 46, 390-397.	3.2	16
98	Electronic structure and properties of YBa ₂ Cu ₄ O ₈ . Physica C: Superconductivity and Its Applications, 1991, 172, 467-476.	1.2	63
99	Coulomb correlated electronic band structure of cuprate superconductors. Physica C: Superconductivity and Its Applications, 1991, 173, 274-284.	1.2	6
100	Normal state transport properties of YBa ₂ Cu ₃ O ₇ and YBa ₂ Cu ₃ O ₈ superconductors; predictions and comparison with experiments. Physica C: Superconductivity and Its Applications, 1991, 176, 159-169.	1.2	45
101	Theoretical two-particle momentum density in YBa ₂ Cu ₃ O ₇ . Journal of Physics and Chemistry of Solids, 1991, 52, 1503-1512.	4.0	12
102	Coulomb correlated band structure and Fermi surfaces of high T _c superconductors. Journal of Physics and Chemistry of Solids, 1991, 52, 1351-1362.	4.0	29
103	Origin of electric-field gradients in high-temperature superconductors: YBa ₂ Cu ₃ O ₇ . Physical Review B, 1991, 43, 532-541.	3.2	61
104	Transport properties of high-T _c superconductors: Fermi-liquid local-density electronic-structure predictions. Physical Review B, 1990, 42, 6238-6243.	3.2	33
105	Calculated photoemission, inverse photoemission, and x-ray emission spectra of high-T _c superconductors: Tl ₂ Ba ₂ CaCu ₂ O ₈ and Tl ₂ Ba ₂ Ca ₂ Cu ₃ O ₁₀ . Physical Review B, 1989, 39, 2894-2897.	3.2	28
106	Electronic structure of Nd-Ce-Cu-O, a Fermi liquid superconductor. Physica C: Superconductivity and Its Applications, 1989, 157, 571-574.	1.2	126
107	Electronic structure and properties of the high-T _c superconductors: Tl ₂ Ba ₂ CaCu ₂ O ₈ and Tl ₂ Ba ₂ Ca ₂ Cu ₃ O ₁₀ . Physica C: Superconductivity and Its Applications, 1988, 152, 273-282.	1.2	116
108	Electronic structure and properties of Bi ₂ Sr ₂ CaCu ₂ O ₈ , the third high-T _c superconductor. Physica C: Superconductivity and Its Applications, 1988, 152, 251-258.	1.2	343

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109	Electronic structure, charge transfer excitations, and high-temperature superconducting oxides (invited). <i>Journal of Applied Physics</i> , 1988, 63, 4220-4225.	2.5	2
110	Calculated photoemission and x-ray emission spectra of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$. <i>Physical Review B</i> , 1988, 38, 5098-5101.	3.2	54
111	Electronic structure and properties of superconducting LiTi_2O_4 . <i>Physical Review B</i> , 1988, 38, 11352-11357.	3.2	64
112	Electronic structure and properties of quasi-two-dimensional layered superconducting perovskites: $\text{La}_{2-x}\text{M}_x\text{CuO}_4$ ($\text{M}=\text{Ba}, \text{Sr}, \dots$). <i>Physical Review B</i> , 1987, 36, 7111-7114.	3.2	49
113	Electronically driven instabilities and superconductivity in the layered $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ perovskites. <i>Physical Review Letters</i> , 1987, 58, 1035-1037.	7.8	544
114	Dominant role of the 2D Van Hove singularity on the Fermi surface and generalized susceptibility of the quasi-2D superconductor $\text{La}_{2-x}\text{M}_x\text{CuO}_4$ ($\text{M} = \text{Sr}, \text{Ba}, \dots$). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1987, 120, 489-493.	2.1	104
115	Calculated local density X-ray and photoemission spectra for superconducting $\text{La}_{2-x}\text{M}_x\text{CuO}_4$: Localization of Cu-3d. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1987, 124, 463-468.	2.1	60
116	Local density theory of X-ray and photoemission from $\text{YBa}_2\text{Cu}_3\text{O}_7$: The high T_c superconductor. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1987, 124, 469-473.	2.1	81
117	Electronic structure and properties of $\text{YBa}_2\text{Cu}_3\text{O}_7$, a low dimensional, low density of states superconductor. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1987, 122, 198-202.	2.1	485
118	Bonds, bands, charge transfer excitations and superconductivity of $\text{YBa}_2\text{Cu}_3\text{O}_7$. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1987, 122, 203-208.	2.1	340
119	All-Electron Local Density Theory of Electronic Structure and Superconductivity in $\text{YBa}_2\text{Cu}_3\text{O}_7$ and $\text{YBa}_2\text{Cu}_3\text{O}_6$. <i>Japanese Journal of Applied Physics</i> , 1987, 26, 1153.	1.5	1