

Jaejun Yu

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	State Induced by Relativistic Spin-Orbit Coupling in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$. Physical Review Letters, 2008, 101, 076402.	7.8	1,332
2	Electronically driven instabilities and superconductivity in the layered $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ perovskites. Physical Review Letters, 1987, 58, 1035-1037.	7.8	544
3	Magnetic ordering at the edges of graphitic fragments: Magnetic tail interactions between the edge-localized states. Physical Review B, 2005, 72, .	3.2	487
4	Electronic structure and properties of $\text{YBa}_2\text{Cu}_3\text{O}_7-\tilde{\tau}$, a low dimensional, low density of states superconductor. Physics Letters, Section A: General, Atomic and Solid State Physics, 1987, 122, 198-202.	2.1	485
5	Electronic structure and properties of $\text{Bi}_2\text{Sr}_2\text{Ca}_\text{Cu}_2\text{O}_8$, the third high-T _c superconductor. Physica C: Superconductivity and Its Applications, 1988, 152, 251-258.	1.2	343
6	Bonds, bands, charge transfer excitations and superconductivity of $\text{YBa}_2\text{Cu}_3\text{O}_7-\tilde{\tau}$. Physics Letters, Section A: General, Atomic and Solid State Physics, 1987, 122, 203-208.	2.1	340
7	Physical properties of transparent perovskite oxides $(\text{Ba},\text{La})\text{SnO}_3$ with high electrical mobility at room temperature. Physical Review B, 2012, 86, .	3.2	264
8	Synthesis, Characterization, and Self-Assembly of Pencil-Shaped CoO Nanorods. Journal of the American Chemical Society, 2006, 128, 9753-9760.	13.7	201
9	Orbital-Angular-Momentum Based Origin of Rashba-Type Surface Band Splitting. Physical Review Letters, 2011, 107, 156803.	7.8	162
10	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
11	Determination of electronic band structures of CaMnO_3 and LaMnO_3 using optical-conductivity analyses. Physical Review B, 1997, 55, 15489-15493.	3.2	134
12	Electronic structure of $\text{Nd}-\text{Ce}-\text{Cu}-\text{O}$, a Fermi liquid superconductor. Physica C: Superconductivity and Its Applications, 1989, 157, 571-574.	1.2	126
13	$\text{O}(\text{N})\text{LDA+U}$ electronic structure calculation method based on the nonorthogonal pseudoatomic orbital basis. Physical Review B, 2006, 73, .	3.2	118
14	Interaction and ordering of vacancy defects in NiO . Physical Review B, 2008, 77, .	3.2	118
15	Anisotropic exchange interactions of spin-orbit-integrated states in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. Physical Review B, 2009, 80, .	3.2	117
16	Electronic structure and properties of the high-T _c superconductors: $\text{Tl}_2\text{Ba}_2\text{Ca}_\text{Cu}_2\text{O}_8$ and $\text{Tl}_2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$. Physica C: Superconductivity and Its Applications, 1988, 152, 273-282.	1.2	116
17	All-perovskite transparent high mobility field effect using epitaxial BaSnO_3 and LaInO_3 . APL Materials, 2015, 3, .	5.1	107
18	Dominant role of the 2D Van Hove singularity on the Fermi surface and generalized susceptibility of the quasi-2D superconductor $\text{La}_{2-x}\text{M}_x\text{CuO}_4$ ($\text{M} = \text{Sr}, \text{Ba}$). Physics Letters, Section A: General, Atomic and Solid State Physics, 1987, 120, 489-493.	2.1	104

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19	ARTICLE on oxygen vacancies and charge carriers induced in the $\langle\text{mml:math}$ xmins:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type interface of a LaAlO $\langle\text{mml:math}$ xmins:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow>/><mml:mn>3</mml:mn></mml:msub></mml:math> overlayer on SrTiO $\langle\text{mml:math}$ xmins:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow>/></mml:msub>	3.2	99
20	Midgap states of La $_{1-x}$ CaxMnO $_3$: Doping-dependent optical-conductivity studies. Physical Review B, 1998, 57, R11043-R11046.	3.2	98
21	Passivated co-doping approach to bandgap narrowing of titanium dioxide with enhanced photocatalytic activity. Applied Catalysis B: Environmental, 2017, 200, 1-9. Topological Quantum Phase Transition in $\langle\text{mml:math}$ xmins:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>5</mml:mn><mml:mi>d</mml:mi></mml:math> Transition Metal Oxide $\langle\text{mml:math}$ xmins:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Na</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>IrO</mml:mi></mml:msub>	20.2	90
22	Physical Review Letters, 2012, 108, 106401.	7.8	87
23	Local density theory of X-ray and photoemission from YBa $_{2-x}$ Cu $_{3-x}$ O $_{7-\delta}$: The high T _c superconductor. Physics Letters, Section A: General, Atomic and Solid State Physics, 1987, 124, 469-473.	2.1	81
24	Electron and Orbital Correlations in Ca $_{2-x}$ SrxRuO $_4$ Probed by Optical Spectroscopy. Physical Review Letters, 2002, 89, 257402.	7.8	77
25	Electronic structures of hexagonal RMnO $_3$ (R=Gd, Tb, Dy, and Ho) thin films: Optical spectroscopy and first-principles calculations. Physical Review B, 2008, 77, .	3.2	75
26	Magnetic ordering and exchange interactions in multiferroic GaFeO $_3$. Physical Review B, 2007, 75, .	3.2	74
27	Spin and orbital angular momentum structure of Cu(111) and Au(111) surface states. Physical Review B, 2012, 85, .	3.2	67
28	Electronic structure and properties of superconducting LiTi $_{2-x}$ O $_4$. Physical Review B, 1988, 38, 11352-11357.	3.2	64
29	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
30	Electronic structure and properties of YBa $_{2-x}$ Cu $_{4-x}$ O $_8$. Physica C: Superconductivity and Its Applications, 1991, 172, 467-476.	1.2	63
31	Origin of electric-field gradients in high-temperature superconductors: YBa $_{2-x}$ Cu $_{3-x}$ O $_{7-\delta}$. Physical Review B, 1991, 43, 532-541.	3.2	61
32	Dopant-site-dependent scattering by dislocations in epitaxial films of perovskite semiconductor BaSnO $_3$. APL Materials, 2014, 2, .	5.1	61
33	Calculated local density X-ray and photoemission spectra for superconducting La $_{2-x}$ M $_x$ CuO $_4$: Localization of Cu-3d. Physics Letters, Section A: General, Atomic and Solid State Physics, 1987, 124, 463-468.	2.1	60
34	Electronic structure, magnetic interactions, and the role of ligands in Mn $_n$ (n=4,12) single-molecule magnets. Physical Review B, 2004, 70, .	3.2	58
35	Calculated photoemission and x-ray emission spectra of Bi $_{2-x}$ Sr $_2$ CaCu $_{2-x}$ O $_8$. Physical Review B, 1988, 38, 5098-5101.	3.2	54
36	Hole states in CuO $_2$ planes and Cu-O chains of YBa $_{2-x}$ Cu $_{3-x}$ O $_{7-\delta}$ and YBa $_{2-x}$ Cu $_{4-x}$ O $_8$ probed by soft-x-ray absorption spectroscopy. Physical Review B, 1992, 45, 2581-2584.	3.2	54

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37	Ab initio study of pentacene on Au(001) surface. <i>Surface Science</i> , 2005, 589, 8-18.	1.9	54
38	Missingxy-Band Fermi Surface in4dTransition-Metal OxideSr ₂ RhO ₄ : Effect of the Octahedra Rotation on the Electronic Structure. <i>Physical Review Letters</i> , 2006, 97, 106401.	7.8	50
39	Electronic structure and properties of quasi-two-dimensional layered superconducting perovskites:La ₂ ^x MxCuO ₄ (M=Ba,Sr,A ⁺). <i>Physical Review B</i> , 1987, 36, 7111-7114.	3.2	49
40	Pseudogap formation in 4 d transition metal oxide BaRuO ₃ . <i>Europhysics Letters</i> , 2001, 55, 280-286.	2.0	48
41	Indications of strong neutral impurity scattering in Ba(Sn,Sb)O ₃ . <i>Physical Review B</i> , 2013, 88, .	3.2	48
42	Normal state transport properties of YBa ₂ Cu ₃ O ₇ and YBa ₂ Cu ₃ O ₈ superconductors; predictions and comparison with experiments. <i>Physica C: Superconductivity and Its Applications</i> , 1991, 176, 159-169.	1.2	45
43	Heat-Induced Transformation of Nanodiamond into a Tube-Shaped Fullerene: A Molecular Dynamics Simulation. <i>Physical Review Letters</i> , 2003, 91, 265701.	7.8	45
44	Effect of Orbital Rotation and Mixing on the Optical Properties of OrthorhombicRMnO ₃ (R=La, Pr, Nd,) T _j ETQq0 0 0 rgBT /Overlock 10 T	7.8	45
45	Ferromagnetism at the edges of the stacked graphitic fragments: an ab initio study. <i>Chemical Physics Letters</i> , 2004, 398, 207-211.	2.6	36
46	Scaling Behavior of Spectral Weight Changes in Perovskite ManganitesLa _{0.7} ^y PryCa _{0.3} MnO ₃ . <i>Physical Review Letters</i> , 1998, 81, 4983-4986.	7.8	35
47	Strain-induced topological insulator phase and effective magnetic interactions in Li ₂ IrO ₃ . <i>Physical Review B</i> , 2013, 87, .	3.2	35
48	Enhanced upper critical fields in a new quasi-one-dimensional superconductor Nb ₂ Pd _x Se ₅ . <i>New Journal of Physics</i> , 2013, 15, 123031.	2.9	35
49	Anomalous spin susceptibility and magnetic polaron formation in the double-exchange systems. <i>Physical Review B</i> , 2000, 61, 9501-9505.	3.2	34
50	Effect of Coulomb Interactions on the Electronic and Magnetic Properties of Two-Dimensional CrSiTe ₃ and CrGeTe ₃ Materials. <i>Journal of Electronic Materials</i> , 2019, 48, 1441-1445.	2.2	34
51	Transport properties of high-T _c superconductors: Fermi-liquid local-density electronic-structure predictions. <i>Physical Review B</i> , 1990, 42, 6238-6243.	3.2	33
52	Tunable magnetic topological insulating phases in monolayer Cr _{1-x} Mn _x 3. <i>Physical Review B</i> , 2018, 98, .	3.2	33
53	Energetics of large carbon clusters:â€¢,â€¢,Crossover from fullerenes to nanotubes. <i>Physical Review B</i> , 2002, 65, .	3.2	32
54	Formation of carbon nanotube semiconductor-metal intramolecular junctions by self-assembly of vacancy defects. <i>Physical Review B</i> , 2007, 76, .	3.2	32

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55	Optical investigations of the charge gap in orbital-ordered La _{1/2} Sr _{3/2} MnO ₄ . Physical Review B, 2000, 61, 6902-6906.	3.2	30
56	Band gap sensitivity of bromine adsorption at carbon nanotubes. Chemical Physics Letters, 2005, 403, 135-139.	2.6	30
57	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
58	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
59	High-k perovskite gate oxide BaHfO ₃ . APL Materials, 2017, 5, .	5.1	28
60	Role of oxygen vacancy in the spin-state change and magnetic ordering in SrCoO ₃ . Physical Review B, 2018, 98, .	3.2	28
61	Spin triplet excitations for a valence bond solid on the kagome lattice. Physical Review B, 2008, 77, .	3.2	23
62	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
63	Catalytic decomposition of acetylene on Fe(001): A first-principles study. Physical Review B, 2002, 66, .	3.2	22
64	A Room-temperature Ferroelectric Ferromagnet in a 1D Tetrahedral Chain Network. Advanced Materials, 2019, 31, e1808104.	21.0	22
65	Pressure-induced phonon softening and electronic topological transition in HgBa ₂ CuO ₄ . Physical Review B, 1996, 54, 1313-1319.	3.2	21
66	Double-exchange model with background superexchange interactions: Phase diagrams of La _{1-x} A _x MnO ₃ manganites. Physical Review B, 1998, 58, 11123-11126.	3.2	21
67	First-principles study of ultrathin (2-2) Gd nanowires encapsulated in carbon nanotubes. Journal of Chemical Physics, 2010, 132, 054701.	3.0	19
68	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
69	Raman modes of the apical oxygen in mercury-based superconductors. Physical Review B, 1995, 52, 15078-15081.	3.2	17
70	Origin of reduced polarizations in short-period BaTiO ₃ /SrTiO ₃ ferroelectric superlattices. Journal of Applied Physics, 2009, 105, .	2.5	17
71	Polarization screening and induced carrier density at the interface of LaAlO ₃ overlayer on SrTiO ₃ (001). Journal of Applied Physics, 2010, 108, .	2.5	17
72	Chern insulator with a nearly flat band in the metal-organic-framework-based Kagome lattice. Scientific Reports, 2019, 9, 13807.	3.3	17

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73	Two-photon momentum density in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$. Physical Review B, 1992, 46, 390-397.	3.2	16	
74	Micro-Raman study of the role of pressure in mercury-based superconductors. Physical Review B, 1995, 51, 644-647.	3.2	16	
75	First-principles effective Hamiltonian for ferroelectric polarization in $\text{BaTiO}_3/\text{SrTiO}_3$ superlattices. Journal of Applied Physics, 2008, 103, 124106.	2.5	15	
76	Possible origins of defect-induced magnetic ordering in carbon-irradiated graphite. Physical Review B, 2009, 79, .	3.2	15	
77	Impact of vacancy clusters on characteristic resistance change of nonstoichiometric strontium titanate nano-film. Applied Physics Letters, 2014, 104, .	3.3	15	
78	Suppression of ferromagnetic ordering in doped manganites: Effects of the superexchange interaction. Physical Review B, 2000, 61, 428-431.	3.2	14	
79	Structure and magnetism of small Gd and Fe nanoclusters: $\text{LDA} + \text{molecular orbital calculations}$. Solid State Communications, 2009, 149, 2058-2060.	1.9	14	
80	Tunable charge donation and spin polarization of metal adsorbates on graphene using an applied electric field. Physical Review B, 2010, 82, .	3.2	13	
81	Mapping Atomic Contact between Pentacene and a Au Surface using Scanning Tunneling Spectroscopy. Nano Letters, 2010, 10, 996-999.	9.1	13	
82	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	
83	Theoretical two-particle momentum density in $\text{YBa}_2\text{Cu}_3\text{O}_7$. Journal of Physics and Chemistry of Solids, 1991, 52, 1503-1512.	4.0	12	
84	Competition between structural distortion and magnetic moment formation in fullerene C ₂₀ . Journal of Chemical Physics, 2009, 130, 184107.	3.0	12	
85	Magnetic interactions in PdCrO_2 and their effects on its magnetic structure. Physical Review B, 2018, 98, .			
86	Electronic structure and properties of vacancy-ordered $\text{YBa}_2\text{Cu}_3\text{O}_6.5$. Physica C: Superconductivity and Its Applications, 1993, 214, 335-344.	1.2	11	
87	Dimensional crossover driven by magnetic ordering in optical conductivity of $\text{Pr}_{1/2}\text{Sr}_{1/2}\text{MnO}_3$. Physical Review B, 2000, 61, 14656-14659.	3.2	11	
88	Enhanced Charge Gap in the Bilayer Manganite $\text{La}_{2-x}\text{Sr}_x\text{Mn}_2\text{O}_7$ near $x=0.4$. Physical Review Letters, 2007, 98, 187201.	7.8	11	
89	Modulation of electron carrier density at the n-type $\text{LaAlO}_3/\text{SrTiO}_3$ interface by water adsorption. Journal of Physics Condensed Matter, 2013, 25, 265004.	1.8	11	
90	Doped valence-bond solid and superconductivity on the Shastry-Sutherland lattice. Physical Review B, 2008, 77, .	3.2	10	

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91	Collinear and noncollinear spin ground state of wurtzite CoO. <i>Physical Review B</i> , 2013, 87, .	3.2	10
92	Charge and magnetic states of rutile TiO ₂ doped with Cr ions. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 146003.	1.8	10
93	Magnetic states and intervalence charge transfer of Ti and Fe defects in $\hat{t}\pm\text{Al}_2\text{O}_3$: The origin of the blue in sapphire. <i>Acta Materialia</i> , 2018, 143, 248-256.	7.9	10
94	Band gap narrowing of TiO ₂ nanoparticles: A passivated Co-doping approach for enhanced photocatalytic activity. <i>Journal of Physics and Chemistry of Solids</i> , 2022, 162, 110503.	4.0	9
95	Electronic band structure of high T _c Cu-oxide superconductors: Comparison of predictions with experiments. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 1994, 66, 281-301.	1.7	7
96	Photonic crystal alloys: a new twist in controlling photonic band structure properties. <i>Optics Express</i> , 2008, 16, 6579.	3.4	7
97	<i>< i>Ab Initio</i> Study of Elastic Properties of High-Pressure Polymorphs of CO<sub>2</sub> Phases II and V.</i> <i>Journal of Physical Chemistry C</i> , 2016, 120, 23152-23164.	3.1	7
98	Coulomb correlated electronic band structure of cuprate superconductors. <i>Physica C: Superconductivity and Its Applications</i> , 1991, 173, 274-284.	1.2	6
99	Induced vortex dynamics in parallel Josephson junction arrays. <i>Physical Review B</i> , 1997, 55, 1231-1235. Interface electronic structure, two-dimensional metallicity, and possible interface superconductivity in<math>\text{mml:math}<\!\!\text{xmlns:mml}=\text{"http://www.w3.org/1998/Math/MathML"}<\!\!><\!\!\text{display}=\text{"inline"}<\!\!\text{>}<\!\!\text{mml:mrow}<\!\!\text{>}<\!\!\text{mml:mi mathvariant}=\text{"normal"}<\!\!\text{>} \text{Cu} <\!\!\text{</mml:mi}<\!\!\text{>} <\!\!\text{mml:mi mathvariant}=\text{"normal"}<\!\!\text{>} \text{Cl} <\!\!\text{</mml:mi}<\!\!\text{>} <\!\!\text{mml:mo} \hat{\wedge} \bullet <\!\!\text{</mml:mo}<\!\!\text{>} <\!\!\text{mml:mi mathvariant}=\text{"normal"}<\!\!\text{>} \text{Si} <\!\!\text{</mml:mi}<\!\!\text{>} <\!\!\text{/mml:mrow}<\!\!\text{>} <\!\!\text{/mml:math}<\!\!> \text{superlattices.} <i>Physical Review B</i> , 2007, 76,	3.2	6
100	Graphene analogue in (111)-oriented BaBiO ₃ bilayer heterostructures for topological electronics. <i>Scientific Reports</i> , 2018, 8, 555.	3.3	6
101	Inevitable high density of oxygen vacancies at the surface of polarâ€“nonpolar perovskite heterostructures LaAlO ₃ /SrTiO ₃ . <i>Journal of Applied Physics</i> , 2020, 127, .	2.5	6
102	Chirality-induced spin texture switching in twisted bilayer graphene. <i>Physical Review B</i> , 2021, 104, .	3.2	5
103	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
104	Superstructures of Se adsorbates on Au(111): Scanning tunneling microscopy and spectroscopy study. <i>Surface Science</i> , 2019, 685, 19-23.	1.9	4
105	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
106	Long-range hopping correlation and colossal magnetoresistance in doped manganites. <i>Journal of Physics Condensed Matter</i> , 2000, 12, 5453-5462.	1.8	3
107	Multiferroic Materials: A Room-Temperature Ferroelectric Ferromagnet in a 1D Tetrahedral Chain Network (<i>Adv. Mater.</i> 24/2019). <i>Advanced Materials</i> , 2019, 31, 1970173.	21.0	3

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109	Band gap and mobility of epitaxial perovskite BaSn _{1-x} HfxO ₃ thin films. Physical Review Materials, 2018, 2, .		2.4	3
110	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
111	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
112	Electronic structure, charge transfer excitations, and high-temperature superconducting oxides (invited). Journal of Applied Physics, 1988, 63, 4220-4225.		2.5	2
113	Optical properties of BaRuO ₃ : observation of pseudogap formation. Current Applied Physics, 2001, 1, 163-167.		2.4	2
114	A spin-dependent local moment approach to the Anderson impurity model. Journal of Physics Condensed Matter, 2007, 19, 456203.		1.8	2
115	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
116	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
117	All-Electron Local Density Theory of Electronic Structure and Superconductivity in YBa ₂ Cu ₃ O ₇ and YBa ₂ Cu ₃ O ₆ . Japanese Journal of Applied Physics, 1987, 26, 1153.		1.5	1
118	Current-voltage characteristics and Josephson ac effects of granular HTSC Y ₁ Ba ₂ Cu ₃ O _y bridges. Solid State Communications, 1995, 94, 45-48.		1.9	0
119	Current Status of Women Physicists in Korea. AIP Conference Proceedings, 2005, , .		0.4	0