Jun-Wei Luo

List of Publications by Year
in descending order

108 papers	3,651 citations	126907 33 h-index	144013 57 g-index
108 all docs	108 docs citations	108 times ranked	5430 citing authors

#	Article	IF	Citations
1	Algorithm advances and applications of timeâ€dependent firstâ€principles simulations for ultrafast dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1577.	14.6	6
2	Progress of hidden spin polarization in inversion-symmetric crystals. Science China: Physics, Mechanics and Astronomy, 2022, 65, 1.	5.1	6
3	Cryogenic Mobility Enhancement in Si MOS Devices via SiO₂ Regrowth. IEEE Transactions on Electron Devices, 2022, 69, 2585-2589.	3.0	4
4	Emergent linear Rashba spin-orbit coupling offers fast manipulation of hole-spin qubits in germanium. Physical Review B, 2022, 105, .	3.2	8
5	Orientation-dependent Rashba spin-orbit coupling of two-dimensional hole gases in semiconductor quantum wells: Linear or cubic. Physical Review B, 2022, 105, .	3.2	5
6	Origin of giant valley splitting in silicon quantum wells induced by superlattice barriers. Physical Review B, 2022, 105, .	3.2	5
7	Low-thermal-budget n-type ohmic contacts for ultrathin Si/Ge superlattice materials. Journal Physics D: Applied Physics, 2022, 55, 355110.	2.8	2
8	Dynamic short-range correlation in photoinduced disorder phase transitions. Physical Review B, 2022, 105, .	3.2	1
9	Prediction of low-Z collinear and noncollinear antiferromagnetic compounds having momentum-dependent spin splitting even without spin-orbit coupling. Physical Review Materials, 2021, 5, .	2.4	64
10	Emergence of strong tunable linear Rashba spin-orbit coupling in two-dimensional hole gases in semiconductor quantum wells. Physical Review B, 2021, 103, .	3.2	24
11	Chiral Mesostructured NiO Films with Spin Polarisation. Angewandte Chemie, 2021, 133, 9507-9512.	2.0	1
12	Chiral Mesostructured NiO Films with Spin Polarisation. Angewandte Chemie - International Edition, 2021, 60, 9421-9426.	13.8	35
13	The critical role of hot carrier cooling in optically excited structural transitions. Npj Computational Materials, 2021, 7, .	8.7	11
14	Group velocity matters for accurate prediction of phonon-limited carrier mobility*. Chinese Physics B, 2021, 30, 087201.	1.4	0
15	Decoupling of the Electrical and Thermal Transports in Strongly Coupled Interlayer Materials. Journal of Physical Chemistry Letters, 2021, 12, 7832-7839.	4.6	8
16	Giant momentum-dependent spin splitting in centrosymmetric low- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Z</mml:mi></mml:math> antiferromagnets. Physical Review B, 2020, 102, .	3.2	101
17	Hidden spin polarization in the centrosymmetric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> crystal revealed via elliptically polarized terahertz emission. Physical Review B, 2020, 102, .	3.2	17
18	Electrically switchable hidden spin polarization in antiferroelectric crystals. Physical Review B, 2020, 102, .	3.2	13

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19	Microscopic force driving the photoinduced ultrafast phase transition: Time-dependent density functional theory simulations of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">IrTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2020, 102, .	3.2	15
20	Image charge interaction correction in charged-defect calculations. Physical Review B, 2020, 102, .	3.2	24
21	Three-Dimensional Mechanistic Modeling of Gate Leakage Current in High- Îº MOSFETs. Physical Review Applied, 2020, 13, .	3.8	4
22	Realistic dimension-independent approach for charged-defect calculations in semiconductors. Physical Review B, 2020, 101, .	3.2	30
23	Interface-engineering enhanced light emission from Si/Ge quantum dots. New Journal of Physics, 2020, 22, 093037.	2.9	5
24	(Invited) Theory of Silicon-Based Light Emitting. ECS Transactions, 2020, 98, 77-89.	0.5	1
25	(Invited) Theory of Silicon-Based Light Emitting. ECS Meeting Abstracts, 2020, MA2020-02, 1719-1719.	0.0	0
26	Digging for topological property in disordered alloys: the emergence of Weyl semimetal phase and sequential band inversions in PbSeâ€“SnSe alloys. Materials Horizons, 2019, 6, 2124-2134.	12.2	15
27	Impurity diffusion induced dynamic electron donors in semiconductors. Physical Review B, 2019, 100, .	3.2	8
28	Revealing angular momentum transfer channels and timescales in the ultrafast demagnetization process of ferromagnetic semiconductors. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19258-19263.	7.1	11
29	[illegible] of Charge Trapping across the Crystalline- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Si</mml:mi></mml:math> â€“Amorphous- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Si</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> Interf	3.8	22
30	Design Principles of p-Type Transparent Conductive Materials. ACS Applied Materials & Interfaces, 2019, 11, 24837-24849.	8.0	35
31	Origin of the anomalous trends in band alignment of GaX/ZnGeX₂ (X = N, P, As, Sb) heterojunctions. Journal of Semiconductors, 2019, 40, 042102.	3.7	10
32	Uncovering and tailoring hidden Rashba spinâ€“orbit splitting in centrosymmetric crystals. Nature Communications, 2019, 10, 906.	12.8	53
33	A systematic study of the negative thermal expansion in zinc-blende and diamond-like semiconductors. New Journal of Physics, 2019, 21, 123015.	2.9	10
34	Characterizing the Charge Trapping across Crystalline and Amorphous Si/SiO ₂ /HfO ₂ Stacks from First-Principle Calculations. Physical Review Applied, 2019, 12, .	3.8	18
35	Alloy theory with atomic resolution for Rashba or topological systems. Physical Review Materials, 2019, 3, .	2.4	3
36	The Pentagonal Nature of Self-Assembled Silicon Chains and Magic Clusters on Ag(110). Nano Letters, 2018, 18, 2937-2942.	9.1	52

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37	Band structure engineering and defect control of oxides for energy applications. Chinese Physics B, 2018, 27, 117104.	1.4	17
38	Unified theory of direct or indirect band-gap nature of conventional semiconductors. Physical Review B, 2018, 98, .	3.2	60
39	Photocorrosion-Limited Maximum Efficiency of Solar Photoelectrochemical Water Splitting. Physical Review Applied, 2018, 10, .	3.8	44
40	Fundamental Intrinsic Lifetimes in Semiconductor Self-Assembled Quantum Dots. Physical Review Applied, 2018, 10, .	3.8	3
41	Atomic-Ordering-Induced Quantum Phase Transition between Topological Crystalline Insulator and Z 2 Topological Insulator. Chinese Physics Letters, 2018, 35, 057301.	3.3	6
42	Improving Performances of In-Plane Transition-Metal Dichalcogenide Schottky Barrier Field-Effect Transistors. ACS Applied Materials & Interfaces, 2018, 10, 19271-19277.	8.0	89
43	Two dimensional Schottky contact structure based on in-plane zigzag phosphorene nanoribbon. Organic Electronics, 2017, 44, 20-24.	2.6	38
44	In-plane Schottky-barrier field-effect transistors based on 1 <i>T</i> /2 <i>H</i> heterojunctions of transition-metal dichalcogenides. Physical Review B, 2017, 96, .	3.2	117
45	Absence of redshift in the direct bandgap of silicon nanocrystals with reduced size. Nature Nanotechnology, 2017, 12, 930-932.	31.5	22
46	Rapid Transition of the Hole Rashba Effect from Strong Field Dependence to Saturation in Semiconductor Nanowires. Physical Review Letters, 2017, 119, 126401.	7.8	21
47	Tunable Electronic Structures of GeSe Nanosheets and Nanoribbons. Journal of Physical Chemistry C, 2017, 121, 14373-14379.	3.1	62
48	Electronic band structure of epitaxial PbTe (111) thin films observed by angle-resolved photoemission spectroscopy. Physical Review B, 2017, 95, .	3.2	6
49	ab initio simulation on mono-layer MoS2 tunnel FET: Impact of metal contact configuration and defect assisted tunneling. , 2016, , .		0
50	Suppress carrier recombination by introducing defects: The case of Si solar cell. Applied Physics Letters, 2016, 108, .	3.3	23
51	Origin of the Distinct Diffusion Behaviors of Cu and Ag in Covalent and Ionic Semiconductors. Physical Review Letters, 2016, 117, 165901.	7.8	25
52	Single-dot absorption spectroscopy and theory of silicon nanocrystals. Physical Review B, 2016, 93, .	3.2	39
53	Strong Absorption Enhancement in Si Nanorods. Nano Letters, 2016, 16, 7937-7941.	9.1	11
54	Revealing the Origin of Fast Electron Transfer in TiO₂-Based Dye-Sensitized Solar Cells. Journal of the American Chemical Society, 2016, 138, 8165-8174.	13.7	54

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55	Quasi-Direct Optical Transitions in Silicon Nanocrystals with Intensity Exceeding the Bulk. Nano Letters, 2016, 16, 1583-1589.	9.1	62
56	How good is mono-layer transition-metal dichalcogenide tunnel field-effect transistors in sub-10 nm? - An ab initio simulation study. , 2015, , .		13
57	Supercoupling between heavy-hole and light-hole states in nanostructures. Physical Review B, 2015, 92, .	3.2	31
58	Zinc-blende and wurtzite GaAs quantum dots in nanowires studied using hydrostatic pressure. Physical Review B, 2015, 92, .	3.2	7
59	The origin of electronic band structure anomaly in topological crystalline insulator group-IV tellurides. Npj Computational Materials, 2015, 1, .	8.7	38
60	Split Dirac cones in HgTe/CdTe quantum wells due to symmetry-enforced level anticrossing at interfaces. Physical Review B, 2015, 91, .	3.2	67
61	Highly sensitive and fast phototransistor based on large size CVD-grown SnS₂nanosheets. Nanoscale, 2015, 7, 14093-14099.	5.6	126
62	Chemical trends of stability and band alignment of lattice-matched II-VI/III-V semiconductor interfaces. Physical Review B, 2015, 91, .	3.2	21
63	Sulfur vacancy activated field effect transistors based on ReS₂nanosheets. Nanoscale, 2015, 7, 15757-15762.	5.6	44
64	Reinterpretation of the Expected Electronic Density of States of Semiconductor Nanowires. Nano Letters, 2015, 15, 88-95.	9.1	9
65	Semiconductor Materials Genome Initiative: silicon-based light emission material. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 207803.	0.5	0
66	Improved quantum dot stacking for intermediate band solar cells using strain compensation. Nanotechnology, 2014, 25, 445402.	2.6	17
67	Statistical properties of exciton fine structure splitting and polarization angles in quantum dot ensembles. Physical Review B, 2014, 89, .	3.2	16
68	Hidden spin polarization in inversion-symmetric bulk crystals. Nature Physics, 2014, 10, 387-393.	16.7	400
69	Origin of the failed ensemble average rule for the band gaps of disordered nonisovalent semiconductor alloys. Physical Review B, 2014, 90, .	3.2	13
70	Mapping the orbital wavefunction of the surface states in three-dimensional topological insulators. Nature Physics, 2013, 9, 499-504.	16.7	118
71	2D optical photon echo spectroscopy of a selfâ€assembled quantum dot. Annalen Der Physik, 2013, 525, 31-42.	2.4	11
72	Self-assembled quantum dots in a nanowire system for quantum photonics. Nature Materials, 2013, 12, 439-444.	27.5	306

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73	Genetic design of enhanced valley splitting towards a spin qubit in silicon. Nature Communications, 2013, 4, 2396.	12.8	49
74	Influence of the atomic-scale structure on the exciton fine-structure splitting in InGaAs and GaAs quantum dots in a vertical electric field. Physical Review B, 2012, 86, .	3.2	17
75	Dissecting biexciton wave functions of self-assembled quantum dots by double-quantum-coherence optical spectroscopy. Physical Review B, 2012, 86, .	3.2	10
76	Genetic-Algorithm Discovery of a Direct-Gap and Optically Allowed Superstructure from Indirect-Gap Si and Ge Semiconductors. Physical Review Letters, 2012, 108, 027401.	7.8	103
77	Quantum mechanical simulations of nano-structures and nano-devices. , 2012, , .		0
78	The Birth of a Type-II Nanostructure: Carrier Localization and Optical Properties of Isoelectronically Doped CdSe:Te Nanocrystals. ACS Nano, 2012, 6, 8325-8334.	14.6	15
79	Genomic Design of Strong Direct-Gap Optical Transition in Si/Ge Core/Multishell Nanowires. Nano Letters, 2012, 12, 984-991.	9.1	54
80	Large insulating gap in topological insulators induced by negative spin-orbit splitting. Physical Review B, 2012, 86, .	3.2	26
81	Strained Interface Defects in Silicon Nanocrystals. Advanced Functional Materials, 2012, 22, 3223-3232.	14.9	63
82	False-positive and false-negative assignments of topological insulators in density functional theory and hybrids. Physical Review B, 2011, 84, .	3.2	93
83	Matrix-embedded silicon quantum dots for photovoltaic applications: a theoretical study of critical factors. Energy and Environmental Science, 2011, 4, 2546.	30.8	72
84	Geometry of epitaxial GaAs/(Al,Ga)As quantum dots as seen by excitonic spectroscopy. Physical Review B, 2011, 84, .	3.2	16
85	Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. Physical Review B, 2011, 84, .	3.2	24
86	Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. Physical Review B, 2011, 84, .	3.2	15
87	Design Principles and Coupling Mechanisms in the 2D Quantum Well Topological InsulatorHgTe/CdTe. Physical Review Letters, 2010, 105, 176805.	7.8	31
88	Discovery of a Novel Linear-in-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>k</mml:mi></mml:math>Spin Splitting for Holes in the 2D<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>GaAs</mml:mi><mml:mo>/</mml:mo><mml:mi>AlAs</mml:mi></mml:math>System. Physical Review Letters, 2010, 104, 066405.	7.8	41
89	Wide InP Nanowires with Wurtzite/Zincblende Superlattice Segments Are Type-II whereas Narrower Nanowires Become Type-I: An Atomistic Pseudopotential Calculation. Nano Letters, 2010, 10, 4055-4060.	9.1	76
90	Origin of one-photon and two-photon optical transitions in PbSe nanocrystals. Physical Review B, 2009, 79, .	3.2	18

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91	Nonmonotonic size dependence of the dark/bright exciton splitting in GaAs nanocrystals. Physical Review B, 2009, 79, .	3.2	20
92	Quantum mechanical simulation of nanosized metal-oxide-semiconductor field-effect transistor using empirical pseudopotentials: A comparison for charge density occupation methods. Journal of Applied Physics, 2009, 106, 084510.	2.5	2
93	Understanding the physics of Carrier-Multiplication and intermediate-band solar cells based on nanostructures - What is going on?. , 2009, , .		1
94	Long- and short-range electronâ€"hole exchange interaction in different types of quantum dots. New Journal of Physics, 2009, 11, 123024.	2.9	19
95	Atomistic pseudopotential calculations of thickness-fluctuation GaAs quantum dots. Physical Review B, 2009, 79, .	3.2	24
96	Full-Zone Spin Splitting for Electrons and Holes in Bulk GaAs and GaSb. Physical Review Letters, 2009, 102, 056405.	7.8	47
97	Direct-Bandgap InAs Quantum-Dots Have Long-Range Electronâˆ'Hole Exchange whereas Indirect Gap Si Dots Have Short-Range Exchange. Nano Letters, 2009, 9, 2648-2653.	9.1	15
98	A Fully Three-Dimensional Atomistic Quantum Mechanical Study on Random Dopant-Induced Effects in 25-nm MOSFETs. IEEE Transactions on Electron Devices, 2008, 55, 1720-1726.	3.0	8
99	Multiple valley couplings in nanometer Si metalâ€"oxideâ€"semiconductor field-effect transistors. Journal of Applied Physics, 2008, 103, 124507.	2.5	4
100	Carrier Multiplication in Semiconductor Nanocrystals: Theoretical Screening of Candidate Materials Based on Band-Structure Effects. Nano Letters, 2008, 8, 3174-3181.	9.1	80
101	Rashba spin splitting of the minibands of coupled InAsâ^•GaAs pyramid quantum dots. Applied Physics Letters, 2008, 92, .	3.3	5
102	Quantum-size-induced electronic transitions in quantum dots: Indirect band-gap GaAs. Physical Review B, 2008, 78, .	3.2	30
103	Chemical trends of defect formation in Si quantum dots: The case of group-III and group-V dopants. Physical Review B, 2007, 75, .	3.2	48
104	Quantum mechanical effects in nanometer field effect transistors. Applied Physics Letters, 2007, 90, 143108.	3.3	9
105	Comparative study for colloidal quantum dot conduction band state calculations. Applied Physics Letters, 2006, 88, 143108.	3.3	15
106	Photoluminescence pressure coefficients ofInAsâ^•GaAsquantum dots. Physical Review B, 2005, 71, .	3.2	32
107	New quantum dot nanomaterials to boost solar energy harvesting. SPIE Newsroom, 0, , .	0.1	4
108	Directly confirming the Z 1/2 center as the electron trap in SiC through accessing the nonâ€radiative recombination. Physica Status Solidi - Rapid Research Letters, 0, , 2100458.	2.4	2