Qun-Xiang Li

List of Publications by Year
in descending order

137 papers	6,568 citations	76326 40 h-index	64796 79 g-index
137 all docs	137 docs citations	137 times ranked	8879 citing authors

#	Article	IF	Citations
1	Controlling the Kondo Effect of an Adsorbed Magnetic Ion Through Its Chemical Bonding. Science, 2005, 309, 1542-1544.	12.6	594
2	Surface Structure-Dependent Molecular Oxygen Activation of BiOCl Single-Crystalline Nanosheets. Journal of the American Chemical Society, 2013, 135, 15750-15753.	13.7	560
3	Co₃O₄ Hexagonal Platelets with Controllable Facets Enabling Highly Efficient Visibleâ€Light Photocatalytic Reduction of CO₂. Advanced Materials, 2016, 28, 6485-6490.	21.0	395
4	Enhanced photocatalytic mechanism for the hybrid g-C₃N₄/MoS₂ nanocomposite. Journal of Materials Chemistry A, 2014, 2, 7960-7966.	10.3	347
5	Facile synthesis of pentacle goldâ€“copper alloy nanocrystals and their plasmonic and catalytic properties. Nature Communications, 2014, 5, 4327.	12.8	294
6	Electronic structures of SiC nanoribbons. Journal of Chemical Physics, 2008, 129, 174114.	3.0	222
7	Graphene nanoribbon as a negative differential resistance device. Applied Physics Letters, 2009, 94, .	3.3	219
8	Metal-like fluorine-doped Î²-FeOOH nanorods grown on carbon cloth for scalable high-performance supercapacitors. Nano Energy, 2015, 11, 119-128.	16.0	184
9	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2008, 129, 074704.	3.0	182
10	Tuning the electronic structure of graphene nanoribbons through chemical edge modification: A theoretical study. Physical Review B, 2007, 75, .	3.2	156
11	Identifying Molecular Orientation of IndividualC60on aSi(111)â˜(7Ã—7)Surface. Physical Review Letters, 1999, 83, 3001-3004.	7.8	135
12	Z-shaped graphene nanoribbon quantum dot device. Applied Physics Letters, 2007, 91, .	3.3	109
13	Irreversible accumulated SERS behavior of the molecule-linked silver and silver-doped titanium dioxide hybrid system. Nature Communications, 2020, 11, 1785.	12.8	107
14	A Highly Efficient Metalâ€Free Electrocatalyst of Fâ€Doped Porous Carbon toward N₂ Electroreduction. Advanced Materials, 2020, 32, e1907690.	21.0	105
15	Epitaxial facet junctions on TiO₂ single crystals for efficient photocatalytic water splitting. Energy and Environmental Science, 2018, 11, 1444-1448.	30.8	102
16	Topology of two-dimensional C60 domains. Nature, 2001, 409, 304-305.	27.8	101
17	Enhanced N₂ Electroreduction over LaCoO₃ by Introducing Oxygen Vacancies. ACS Catalysis, 2020, 10, 1077-1085.	11.2	98
18	Band Structure Tuning of TiO₂ for Enhanced Photoelectrochemical Water Splitting. Journal of Physical Chemistry C, 2014, 118, 7451-7457.	3.1	95

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19	Chiral selective tunneling induced negative differential resistance in zigzag graphene nanoribbon: A theoretical study. Applied Physics Letters, 2008, 92, .	3.3	93
20	Green Eu2+-doped Ba3Si6O12N2 phosphor for white light-emitting diodes: Synthesis, characterization and theoretical simulation. Journal of Luminescence, 2011, 131, 1101-1106.	3.1	83
21	Electronic and magnetic properties of V-doped anataseTiO2from first principles. Physical Review B, 2006, 74, .	3.2	80
22	Single-layer cadmium chalcogenides: promising visible-light driven photocatalysts for water splitting. Physical Chemistry Chemical Physics, 2016, 18, 17029-17036.	2.8	75
23	Orientational configurations of theC60molecules in the(2Ã—2)superlattice on a solidC60(111) surface at low temperature. Physical Review B, 2001, 63, .	3.2	66
24	Unveiling Metal-Cage Hybrid States in a Single Endohedral Metallofullerene. Physical Review Letters, 2003, 91, 185504.	7.8	61
25	Titanium/Yttrium Mixed Metal Nitride Clusterfullerene TiY₂N@C₈₀: Synthesis, Isolation, and Effect of the Group-III Metal. Inorganic Chemistry, 2012, 51, 3039-3045.	4.0	61
26	Evidence of van Hove Singularities in Ordered Grain Boundaries of Graphene. Physical Review Letters, 2014, 112, 226802.	7.8	61
27	Entrapping a Group-VB Transition Metal, Vanadium, within an Endohedral Metallofullerene: V_xSc_{3â€“x}N@I_h-C₈₀ (x = 1, 2). Journal of the American Chemical Society, 2016, 138, 207-214.	13.7	60
28	Nonequilibrium electronic transport of 4,4â€²-bipyridine molecular junction. Journal of Chemical Physics, 2005, 123, 184712.	3.0	59
29	Single- and few-layer BiOI as promising photocatalysts for solar water splitting. RSC Advances, 2017, 7, 24446-24452.	3.6	59
30	Iron-phthalocyanine molecular junction with high spin filter efficiency and negative differential resistance. Journal of Chemical Physics, 2012, 136, 064707.	3.0	58
31	Ballistic rectification in a Z-shaped graphene nanoribbon junction. Applied Physics Letters, 2008, 92, .	3.3	55
32	Average density of states in disordered graphene systems. Physical Review B, 2008, 77, .	3.2	54
33	Low-Temperature Orientationally Ordered Structures of Two-Dimensional C60. Journal of the American Chemical Society, 2003, 125, 169-172.	13.7	53
34	First-principles study ofNi2P(0001) surfaces. Physical Review B, 2006, 74, .	3.2	52
35	Carbon Tetragons as Definitive Spin Switches in Narrow Zigzag Graphene Nanoribbons. Physical Review Letters, 2016, 116, 026802.	7.8	51
36	Electrochemical activity of 1Tâ€² structured rhenium selenide nanosheets via electronic structural modulation from selenium-vacancy generation. Journal of Materials Chemistry A, 2018, 6, 22526-22533.	10.3	49

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37	Tuning the coordination number of Fe single atoms for the efficient reduction of CO₂. Green Chemistry, 2020, 22, 7529-7536.	9.0	49
38	Structurally ordered intermetallic Ir3V electrocatalysts for alkaline hydrogen evolution reaction. Nano Energy, 2021, 81, 105636.	16.0	45
39	Switching mechanism of photochromic diarylethene derivatives molecular junctions. Journal of Chemical Physics, 2007, 127, 094705.	3.0	44
40	Tuning the Doping Types in Graphene Sheets by N Monoelement. Nano Letters, 2018, 18, 386-394.	9.1	44
41	Efficient organometallic spin filter based on Europium-cyclooctatetraene wire. Journal of Chemical Physics, 2009, 131, .	3.0	43
42	Scanning tunneling spectroscopy of individual C60 molecules adsorbed on Si(111)-7Ã—7 surface. Surface Science, 1999, 442, L1024-L1028.	1.9	42
43	Tin Oxide Crystals Exposed by Low-Energy {110} Facets for Enhanced Electrochemical Heavy Metal Ions Sensing: X-ray Absorption Fine Structure Experimental Combined with Density-Functional Theory Evidence. Analytical Chemistry, 2017, 89, 2613-2621.	6.5	39
44	Interfacial coupling induced direct Z-scheme water splitting in metal-free photocatalyst: C₃N/g-C₃N₄ heterojunctions. Nanotechnology, 2018, 29, 365401.	2.6	39
45	Coherent transport through spin-crossover magnet Fe₂complexes. Nanoscale, 2016, 8, 609-616.	5.6	37
46	Periodically Modulated Electronic Properties of the Epitaxial Monolayer Graphene on Ru(0001). Journal of Physical Chemistry C, 2011, 115, 24858-24864.	3.1	36
47	Electronic structure of bilayer graphene: A real-space Greenâ€™s function study. Physical Review B, 2007, 75, .	3.2	35
48	Tunable Electronic and Magnetic Properties of Graphene Flake-Doped Boron Nitride Nanotubes. Journal of Physical Chemistry C, 2014, 118, 28616-28624.	3.1	35
49	Linear Band-Gap Modulation of Graphane Nanoribbons under Uniaxial Elastic Strain: A Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 9356-9359.	3.1	32
50	Double-hole codoped huge-gap semiconductor ZrO₂ for visible-light photocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 17517-17524.	2.8	32
51	Band structure engineering of anatase TiO2 by metal-assisted P-O coupling. Journal of Chemical Physics, 2014, 140, 174705.	3.0	29
52	First-Principles Simulation of Scanning Tunneling Microscopy Images of Individual Molecules in Alkanethiol Self-Assembled Monolayers on Au(111). Journal of Physical Chemistry B, 2003, 107, 972-984.	2.6	28
53	Î²-SnS/GaSe heterostructure: a promising solar-driven photocatalyst with low carrier recombination for overall water splitting. Journal of Materials Chemistry A, 2022, 10, 3443-3453.	10.3	28
54	Negative differential resistance devices by using N-doped graphene nanoribbons. Journal of Chemical Physics, 2014, 140, 164703.	3.0	27

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55	Enhanced photoelectrochemical performance of anatase TiO₂ for water splitting via surface codoping. RSC Advances, 2017, 7, 39877-39884.	3.6	25
56	g-C3N4/SnS2 Heterostructure: a Promising Water Splitting Photocatalyst. Chinese Journal of Chemical Physics, 2017, 30, 36-42.	1.3	25
57	Electronic, Magnetic, and Transport Properties of Fe-COT Clusters: A Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 11946-11950.	3.1	24
58	Computational study of the electronic, optical and photocatalytic properties of single-layer hexagonal zinc chalcogenides. Computational Materials Science, 2018, 150, 432-438.	3.0	24
59	Nickel dual-atom catalysts for the selective electrocatalytic debromination of tribromoacetic acid as a green chemistry process. Chemical Engineering Journal, 2022, 427, 131719.	12.7	24
60	A theoretical study of spin-polarized transport properties of planar four-coordinate Fe complexes. Chemical Physics Letters, 2012, 539-540, 102-106.	2.6	23
61	The photoluminescence of Ce-doped Lu4Si2O7N2 green phosphors. Materials Chemistry and Physics, 2009, 118, 270-272.	4.0	22
62	Metal-Free Magnetism and Half-Metallicity of Carbon Nitride Nanotubes: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 22491-22498.	3.1	22
63	Anatase TiO2 codoping with sulfur and acceptor IIB metals for water splitting. International Journal of Hydrogen Energy, 2016, 41, 13050-13057.	7.1	22
64	Rectifying Effect in Polar Conjugated Molecular Junctions: A First-Principles Study. Journal of Nanoscience and Nanotechnology, 2009, 9, 774-778.	0.9	20
65	Thgraphene: a novel two-dimensional carbon allotrope as a potential multifunctional material for electrochemical water splitting and potassium-ion batteries. Journal of Materials Chemistry A, 2022, 10, 9848-9857.	10.3	20
66	Single quintuple bond [PhCrCrPh] molecule as a possible molecular switch. Journal of Chemical Physics, 2006, 125, 184713.	3.0	19
67	Transport properties through diarylethene derivatives between carbon nanotube electrodes: A theoretical study. Chemical Physics Letters, 2009, 479, 120-124.	2.6	19
68	Optimization mechanism of CaSi₂O₂N₂â€‰:â€‰Eu²⁺phosphor by La³⁺ion doping. Journal Physics D: Applied Physics, 2011, 44, 355403.	2.8	19
69	Accurate Determination of the Quasiparticle and Scaling Properties Surrounding the Quantum Critical Point of Disordered Three-Dimensional Dirac Semimetals. Physical Review Letters, 2017, 118, 146401.	7.8	19
70	Blending Nonâ€Groupâ€3 Transition Metal and Rareâ€Earth Metal into a C₈₀ Fullerene Cage with D₅h Symmetry. Angewandte Chemie - International Edition, 2018, 57, 10273-10277.	13.8	18
71	Electronic and optical properties of TiO2 nanotubes and arrays: a first-principles study. Physical Chemistry Chemical Physics, 2014, 16, 11519.	2.8	17
72	C₇N₆/Sc₂CCl₂ Weak van der Waals Heterostructure: A Promising Visible-Light-Driven Z-Scheme Water Splitting Photocatalyst with Interface Ultrafast Carrier Recombination. Journal of Physical Chemistry Letters, 2022, 13, 1473-1479.	4.6	16

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73	Electronic transport property of 4,4â€²-bipyridine molecular junction. Ultramicroscopy, 2005, 105, 293-298.	1.9	15
74	Efficient spin filter based on FeN₄complexes between carbon nanotube electrodes. Nanotechnology, 2012, 23, 255202.	2.6	15
75	Transport spin polarization of magnetic C28 molecular junctions. Chemical Physics Letters, 2012, 535, 111-115.	2.6	15
76	Spin-Crossover and Coherent Transport Behaviors of a Six-Coordinate Iron(II) Complex with a N₄O₂ Donor Set. Journal of Physical Chemistry C, 2019, 123, 16366-16372.	3.1	15
77	A theoretical investigation of GenSn (n=1â€“4) clusters. Computational and Theoretical Chemistry, 2003, 624, 257-265.	1.5	14
78	Achieving indirectâ€toâ€direct band gap transition and enhanced photocatalytic performance in blue phosphorene through doping and strain. International Journal of Quantum Chemistry, 2020, 120, e26230.	2.0	14
79	Electronic transport properties ofPdâ€Hjunctions between twoPdHx(x=0,0.25,0.5,0.75,1)electrodes: A nonequilibrium Greenâ€™s function study. Physical Review B, 2005, 72, .	3.2	13
80	Singly Bonded Monoadduct rather than Methanofullerene: Manipulating the Addition Pattern of Trimetallic Nitride Clusterfullerene through One Endohedral Metal Atom Substitution. Chemistry - A European Journal, 2016, 22, 8309-8315.	3.3	13
81	Assignment of photoelectron spectra of (TiO2)n with n=1â€“3. Journal of Chemical Physics, 2009, 130, 174308.	3.0	12
82	Synthesis and characterization of a multi-functional onâ€“offâ€“on fluorescent oxidized graphitic carbon nitride nanosensor for iodide, chromium(<scp>vi</scp>), and ascorbic acid. Journal of Materials Chemistry C, 2019, 7, 11896-11902.	5.5	12
83	Doubleâ€holeâ€mediated coupling of anionic dopants in perovskite NaNbO₃ for efficient solar water splitting. International Journal of Quantum Chemistry, 2019, 119, e25930.	2.0	11
84	Electronic structure of Ti2AlNb (O phase). Journal of Physics Condensed Matter, 1999, 11, 6179-6186.	1.8	10
85	Orbital-selective single molecule rectifier on graphene-covered Ru(0001) surface. Applied Physics Letters, 2013, 102, 163506.	3.3	10
86	Transport property of ligand-driven light-induced spin-change Fe-based spin crossover complexes. RSC Advances, 2019, 9, 12339-12345.	3.6	10
87	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie - International Edition, 2022, 61, .	13.8	9
88	A first-principles study of acetylene and its evolution products on Cu(001). Journal of Chemical Physics, 2002, 116, 3104-3108.	3.0	8
89	Quantum Dot Based on Z-shaped Graphene Nanoribbon: First-principles Study. Chinese Journal of Chemical Physics, 2007, 20, 489-494.	1.3	8
90	Abnormal growth kinetics of h-BN epitaxial monolayer on Ru(0001) enhanced by subsurface Ar species. Applied Physics Letters, 2018, 112, 171601.	3.3	8

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91	Nanoscale AgInTe2/Si Truncated Quasitetrahedrons for Heterostructured Photodetectors. ACS Applied Nano Materials, 2021, 4, 5785-5795.	5.0	8
92	Computational identification of B substitutional doped C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg"><mml:msub><mml:mrow /><mml:mn>9</mml:mn></mml:msub></mml:math>N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.svg"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math> monolayer for electrocatalytic N<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si10.svg"><mml:msub><mml:mrow /><mml:mml:	2.0	8
93	Houet al.Reply:. Physical Review Letters, 2000, 85, 2654-2654.	7.8	7
94	Protonation effects on electron transport through diblock molecular junctions: A theoretical study. Science in China Series B: Chemistry, 2008, 51, 1159-1165.	0.8	7
95	Carrier-tunable magnetism of graphene with single-atom vacancy. Journal of Applied Physics, 2013, 113, 213709.	2.5	7
96	Structural and electronic properties of an ordered grain boundary formed by separated (1,0) dislocations in graphene. Nanoscale, 2015, 7, 3055-3059.	5.6	7
97	Electronic Transport Properties of Spin-Crossover Magnet Fe(II)-N4S2 Complexes. Chinese Journal of Chemical Physics, 2018, 31, 33-38.	1.3	7
98	Metal to marginal-metal transition in two-dimensional ferromagnetic electron gases. Physical Review B, 2019, 100, .	3.2	7
99	Theoretical investigation of spin-crossover temperature and transport properties of two Fe(II) mononuclear complexes. Chemical Physics Letters, 2020, 758, 137925.	2.6	7
100	Non-Collinear Orbital-induced Planar Quantum Anomalous Hall Effect. Nano Letters, 2020, 20, 7606-7612.	9.1	7
101	Are In13M (M = Li, Na, K) magic clusters? â€“ A comparison with Al13M. Chemical Physics Letters, 2009, 484, 18-23.	2.6	6
102	Impact of Oxygen Vacancy on Band Structure Engineering of n-p Codoped Anatase TiO2. Chinese Journal of Chemical Physics, 2015, 28, 155-160.	1.3	6
103	Spin-Transport Tuning of Individual Magnetic Mn-Salophen Molecule via Chemical Adsorption. Molecules, 2019, 24, 1747.	3.8	6
104	First-principles Study of Single Tin-phthalocyanine Molecule on Ag(111) Surface. Chinese Journal of Chemical Physics, 2010, 23, 565-569.	1.3	5
105	Band-gap engineering in fluorographene nanoribbons under uniaxial strain. Journal of Applied Physics, 2014, 115, 044305.	2.5	5
106	Two-dimensional GaTe/Bi2Se3 heterostructure: A promising direct Z-scheme water splitting photocatalyst. Chinese Journal of Chemical Physics, 2020, 33, 427-433.	1.3	5
107	Bipolar semiconductor in two-dimensional covalent organic frameworks. Physical Review B, 2022, 105, .	3.2	5
108	First-principles investigation forM(CO)n/Ag(110)(M=Fe,Co, Ni, Cu, Zn, and Ag;n=1,2) systems:â€ƒGeometries, STM images, and vibrational frequencies. Physical Review B, 2001, 65, .	3.2	4

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109	First-principles Study of Electron Transport Through Oligoacenes. Chinese Journal of Chemical Physics, 2009, 22, 7-12.	1.3	4
110	ELECTRONIC, MAGNETIC, AND MECHANICAL PROPERTIES OF LINE-DEFECT EMBEDDED GRAPHENE NANORIBBONS: A FIRST-PRINCIPLES STUDY. Nano LIFE, 2012, 02, 1240003.	0.9	4
111	Topological phase transition driven by a spatially periodic potential. Physical Review B, 2014, 90, .	3.2	4
112	Blending Nonâ€Groupâ€3 Transition Metal and Rareâ€Earth Metal into a C₈₀ Fullerene Cage with D₅h</sub> Symmetry. Angewandte Chemie, 2018, 130, 10430-10434.	2.0	4
113	Quantum conductivity correction in a two-dimensional disordered pseudospin-1 system. Physical Review B, 2019, 99, .	3.2	4
114	Pair-Hopping Characteristic of Lithium Diffusive Motion in Li-Doped Î²-Phase Manganese Phthalocyanine. Journal of Physical Chemistry B, 2007, 111, 10064-10068.	2.6	3
115	ELECTRONIC AND STERIC MECHANISMS IN MONO- AND DOUBLE-FLUORINATION OF Cs-C60Cl6. Modern Physics Letters B, 2008, 22, 2727-2738.	1.9	3
116	Coexistence of metallic and insulating-like states in graphene. Scientific Reports, 2015, 5, 8974.	3.3	3
117	Transport properties of a three-shell icosahedral matryoshka cluster: a first-principles study. RSC Advances, 2017, 7, 12704-12710.	3.6	3
118	N₂ Electroreduction: A Highly Efficient Metalâ€Free Electrocatalyst of Fâ€Doped Porous Carbon toward N₂ Electroreduction (Adv. Mater. 24/2020). Advanced Materials, 2020, 32, 2070186.	21.0	3
119	Spin-orbit related power-law dependence of the diffusive conductivity on the carrier density in disordered Rashba two-dimensional electron systems. Physical Review B, 2020, 101, .	3.2	3
120	Lowâ€Temperature Growth of Highâ€Quality Ag₂HgS₂ Crystals for Setup of Weakâ€Light UVâ€“Visibleâ€“NIR Photodetectors. Advanced Optical Materials, 2021, 9, 2002080.	7.3	3
121	TRANSPORT PROPERTY OF TWO ISOELECTRONIC MOLECULES. International Journal of Nanoscience, 2006, 05, 841-846.	0.7	2
122	Chiral selective tunneling induced graphene nanoribbon switch. Frontiers of Physics in China, 2009, 4, 373-377.	1.0	2
123	First-principles Study on the Electronic Structure of Novel Titanium Yttrium Mixed-metal Nitride Clusterfullerene. Chinese Journal of Chemical Physics, 2011, 24, 439-443.	1.3	2
124	Spin-polarized transport properties of Mn@Au6 cluster. Chemical Physics Letters, 2013, 590, 111-115.	2.6	2
125	Negative Differential Resistance and Spin-Filtering Effects in Zigzag Graphene Nanoribbons with Nitrogen-Vacancy Defects. Chinese Journal of Chemical Physics, 2014, 27, 653-658.	1.3	2
126	Phosphorene-based van der Waals heterojunction for solar water splitting. Chinese Journal of Chemical Physics, 2019, 32, 431-436.	1.3	2

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127	Hybrid density functional study on band structure engineering of ZnS(110) surface by anionâ€“cation codoping for overall water splitting. New Journal of Chemistry, 0, , .	2.8	2
128	Theoretical insights into the diverse and tunable charge transport behavior of stilbene-based single-molecule junctions. Chemical Physics, 2022, 556, 111478.	1.9	2
129	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie, 2022, 134, .	2.0	2
130	First-principles simulation of scanning tunneling microscopy images of individual molecules in alkanethiol self-assembled monolayers on Au(111). , 2003, , .		1
131	POLARIZABILITY AND SHIELDING OF COAXIAL HYBRID DOUBLE-WALLED NANOTUBES: A FIRST-PRINCIPLES STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 793-803.	1.8	1
132	Tuning the Electronic Properties of N@C₆₀ Molecule: A Theoretical Study. Journal of Nanoscience and Nanotechnology, 2013, 13, 1053-1058.	0.9	1
133	In-gap localized states induced by adsorbates on silicene. Physical Review B, 2016, 93, .	3.2	1
134	Coherent spin transport through a six-coordinate FeN6 spin-crossover complex with two different spin configurations. Chinese Journal of Chemical Physics, 2019, 32, 579-585.	1.3	1
135	Huge tunneling magnetoresistance in magnetic tunnel junction with Heusler alloy Co2MnSi electrodes. Chinese Journal of Chemical Physics, 2021, 34, 273-280.	1.3	1
136	Coupling effect on the Berry phase. AIP Advances, 2016, 6, 115103.	1.3	0
137	Magnetic field independent shape of the zero-energy landau levels in a disordered T₃ model. New Journal of Physics, 2019, 21, 073013.	2.9	0