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	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
2	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
3	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
4	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
5	Theoretical insights into the diverse and tunable charge transport behavior of stilbene-based single-molecule junctions. Chemical Physics, 2022, 556, 111478.	1.9	2
6	Bipolar semiconductor in two-dimensional covalent organic frameworks. Physical Review B, 2022, 105, .	3.2	5
7	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie - International Edition, 2022, 61, .	13.8	9
8	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie, 2022, 134, .	2.0	2
9	Structurally ordered intermetallic Ir3V electrocatalysts for alkaline hydrogen evolution reaction. Nano Energy, 2021, 81, 105636.	16.0	45
10	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
11	Nanoscale AgInTe2/Si Truncated Quasitetrahedrons for Heterostructured Photodetectors. ACS Applied Nano Materials, 2021, 4, 5785-5795.	5.0	8
12	Huge tunneling magnetoresistance in magnetic tunnel junction with Heusler alloy Co2MnSi electrodes. Chinese Journal of Chemical Physics, 2021, 34, 273-280.	1.3	1
13	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 />	2.0	8
14	Enhanced N₂ Electroreduction over LaCoO₃ by Introducing Oxygen Vacancies. ACS Catalysis, 2020, 10, 1077-1085.	11.2	98
15	Theoretical investigation of spin-crossover temperature and transport properties of two Fe(II) mononuclear complexes. Chemical Physics Letters, 2020, 758, 137925.	2.6	7
16	Tuning the coordination number of Fe single atoms for the efficient reduction of CO₂. Green Chemistry, 2020, 22, 7529-7536.	9.0	49
17	Non-Collinear Orbital-induced Planar Quantum Anomalous Hall Effect. Nano Letters, 2020, 20, 7606-7612.	9.1	7
18	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

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19	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
20	A Highly Efficient Metalâ€Free Electrocatalyst of Fâ€Doped Porous Carbon toward N₂ Electroreduction. Advanced Materials, 2020, 32, e1907690.	21.0	105
21	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
22	Irreversible accumulated SERS behavior of the molecule-linked silver and silver-doped titanium dioxide hybrid system. Nature Communications, 2020, 11, 1785.	12.8	107
23	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
24	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
25	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
26	Spin-Transport Tuning of Individual Magnetic Mn-Salophen Molecule via Chemical Adsorption. Molecules, 2019, 24, 1747.	3.8	6
27	Transport property of ligand-driven light-induced spin-change Fe-based spin crossover complexes. RSC Advances, 2019, 9, 12339-12345.	3.6	10
28	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
29	Quantum conductivity correction in a two-dimensional disordered pseudospin-1 system. Physical Review B, 2019, 99, .	3.2	4
30	Phosphorene-based van der Waals heterojunction for solar water splitting. Chinese Journal of Chemical Physics, 2019, 32, 431-436.	1.3	2
31	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
32	Metal to marginal-metal transition in two-dimensional ferromagnetic electron gases. Physical Review B, 2019, 100, .	3.2	7
33	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
34	Epitaxial facet junctions on TiO₂ single crystals for efficient photocatalytic water splitting. Energy and Environmental Science, 2018, 11, 1444-1448.	30.8	102
35	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
36	Tuning the Doping Types in Graphene Sheets by N Monoelement. Nano Letters, 2018, 18, 386-394.	9.1	44

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37	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
38	Blending Nonâ€Groupâ€3 Transition Metal and Rareâ€Earth Metal into a C₈₀ Fullerene Cage with D₅h Symmetry. Angewandte Chemie, 2018, 130, 10430-10434.	2.0	4
39	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
40	Electronic Transport Properties of Spin-Crossover Magnet Fe(II)-N4S2 Complexes. Chinese Journal of Chemical Physics, 2018, 31, 33-38.	1.3	7
41	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
42	Interfacial coupling induced direct Z-scheme water splitting in metal-free photocatalyst: C₃N/g-C₃N₄ heterojunctions. Nanotechnology, 2018, 29, 365401.	2.6	39
43	Transport properties of a three-shell icosahedral matryoshka cluster: a first-principles study. RSC Advances, 2017, 7, 12704-12710.	3.6	3
44	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
45	Single- and few-layer BiOI as promising photocatalysts for solar water splitting. RSC Advances, 2017, 7, 24446-24452.	3.6	59
46	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
47	Enhanced photoelectrochemical performance of anatase TiO₂ for water splitting via surface codoping. RSC Advances, 2017, 7, 39877-39884.	3.6	25
48	g-C3N4/SnS2 Heterostructure: a Promising Water Splitting Photocatalyst. Chinese Journal of Chemical Physics, 2017, 30, 36-42.	1.3	25
49	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
50	Co₃O₄ Hexagonal Platelets with Controllable Facets Enabling Highly Efficient Visibleâ€Light Photocatalytic Reduction of CO₂. Advanced Materials, 2016, 28, 6485-6490.	21.0	395
51	Coupling effect on the Berry phase. AIP Advances, 2016, 6, 115103.	1.3	0
52	Single-layer cadmium chalcogenides: promising visible-light driven photocatalysts for water splitting. Physical Chemistry Chemical Physics, 2016, 18, 17029-17036.	2.8	75
53	Carbon Tetragons as Definitive Spin Switches in Narrow Zigzag Graphene Nanoribbons. Physical Review Letters, 2016, 116, 026802.	7.8	51
54	Anatase TiO2 codoping with sulfur and acceptor IIB metals for water splitting. International Journal of Hydrogen Energy, 2016, 41, 13050-13057.	7.1	22

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55	Double-hole codoped huge-gap semiconductor ZrO₂ for visible-light photocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 17517-17524.	2.8	32
56	Coherent transport through spin-crossover magnet Fe₂complexes. Nanoscale, 2016, 8, 609-616.	5.6	37
57	In-gap localized states induced by adsorbates on silicene. Physical Review B, 2016, 93, .	3.2	1
58	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
59	Coexistence of metallic and insulating-like states in graphene. Scientific Reports, 2015, 5, 8974.	3.3	3
60	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
61	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
62	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
63	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
64	Tunable Electronic and Magnetic Properties of Graphene Flake-Doped Boron Nitride Nanotubes. Journal of Physical Chemistry C, 2014, 118, 28616-28624.	3.1	35
65	Topological phase transition driven by a spatially periodic potential. Physical Review B, 2014, 90, .	3.2	4
66	Band structure engineering of anatase TiO2 by metal-assisted P-O coupling. Journal of Chemical Physics, 2014, 140, 174705.	3.0	29
67	Negative differential resistance devices by using N-doped graphene nanoribbons. Journal of Chemical Physics, 2014, 140, 164703.	3.0	27
68	Band-gap engineering in fluorographene nanoribbons under uniaxial strain. Journal of Applied Physics, 2014, 115, 044305.	2.5	5
69	Enhanced photocatalytic mechanism for the hybrid g-C₃N₄/MoS₂ nanocomposite. Journal of Materials Chemistry A, 2014, 2, 7960-7966.	10.3	347
70	Electronic and optical properties of TiO2 nanotubes and arrays: a first-principles study. Physical Chemistry Chemical Physics, 2014, 16, 11519.	2.8	17
71	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
72	Facile synthesis of pentacle goldâ€“copper alloy nanocrystals and their plasmonic and catalytic properties. Nature Communications, 2014, 5, 4327.	12.8	294

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73	Band Structure Tuning of TiO₂ for Enhanced Photoelectrochemical Water Splitting. Journal of Physical Chemistry C, 2014, 118, 7451-7457.	3.1	95
74	Evidence of van Hove Singularities in Ordered Grain Boundaries of Graphene. Physical Review Letters, 2014, 112, 226802.	7.8	61
75	Spin-polarized transport properties of Mn@Au6 cluster. Chemical Physics Letters, 2013, 590, 111-115.	2.6	2
76	Surface Structure-Dependent Molecular Oxygen Activation of BiOCl Single-Crystalline Nanosheets. Journal of the American Chemical Society, 2013, 135, 15750-15753.	13.7	560
77	Orbital-selective single molecule rectifier on graphene-covered Ru(0001) surface. Applied Physics Letters, 2013, 102, 163506.	3.3	10
78	Carrier-tunable magnetism of graphene with single-atom vacancy. Journal of Applied Physics, 2013, 113, 213709.	2.5	7
79	Tuning the Electronic Properties of N@C₆₀ Molecule: A Theoretical Study. Journal of Nanoscience and Nanotechnology, 2013, 13, 1053-1058.	0.9	1
80	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
81	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
82	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
83	Efficient spin filter based on FeN₄complexes between carbon nanotube electrodes. Nanotechnology, 2012, 23, 255202.	2.6	15
84	Iron-phthalocyanine molecular junction with high spin filter efficiency and negative differential resistance. Journal of Chemical Physics, 2012, 136, 064707.	3.0	58
85	ELECTRONIC, MAGNETIC, AND MECHANICAL PROPERTIES OF LINE-DEFECT EMBEDDED GRAPHENE NANORIBBONS: A FIRST-PRINCIPLES STUDY. Nano LIFE, 2012, 02, 1240003.	0.9	4
86	Transport spin polarization of magnetic C28 molecular junctions. Chemical Physics Letters, 2012, 535, 111-115.	2.6	15
87	Periodically Modulated Electronic Properties of the Epitaxial Monolayer Graphene on Ru(0001). Journal of Physical Chemistry C, 2011, 115, 24858-24864.	3.1	36
88	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
89	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
90	Optimization mechanism of CaSi₂O₂N₂â€‰:â€‰Eu²⁺phosphor by La³⁺ion doping. Journal Physics D: Applied Physics, 2011, 44, 355403.	2.8	19

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91	First-principles Study of Single Tin-phthalocyanine Molecule on Ag(111) Surface. Chinese Journal of Chemical Physics, 2010, 23, 565-569.	1.3	5
92	Electronic, Magnetic, and Transport Properties of Fe-COT Clusters: A Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 11946-11950.	3.1	24
93	Assignment of photoelectron spectra of (TiO2)n with n=1â€“3. Journal of Chemical Physics, 2009, 130, 174308.	3.0	12
94	First-principles Study of Electron Transport Through Oligoacenes. Chinese Journal of Chemical Physics, 2009, 22, 7-12.	1.3	4
95	Efficient organometallic spin filter based on Europium-cyclooctatetraene wire. Journal of Chemical Physics, 2009, 131, .	3.0	43
96	The photoluminescence of Ce-doped Lu4Si2O7N2 green phosphors. Materials Chemistry and Physics, 2009, 118, 270-272.	4.0	22
97	Are In13M (M = Li, Na, K) magic clusters? â€“ A comparison with Al13M. Chemical Physics Letters, 2009, 484, 18-23.	2.6	6
98	Chiral selective tunneling induced graphene nanoribbon switch. Frontiers of Physics in China, 2009, 4, 373-377.	1.0	2
99	Transport properties through diarylethene derivatives between carbon nanotube electrodes: A theoretical study. Chemical Physics Letters, 2009, 479, 120-124.	2.6	19
100	Graphene nanoribbon as a negative differential resistance device. Applied Physics Letters, 2009, 94, .	3.3	219
101	Rectifying Effect in Polar Conjugated Molecular Junctions: A First-Principles Study. Journal of Nanoscience and Nanotechnology, 2009, 9, 774-778.	0.9	20
102	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
103	Electronic structures of SiC nanoribbons. Journal of Chemical Physics, 2008, 129, 174114.	3.0	222
104	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2008, 129, 074704.	3.0	182
105	Ballistic rectification in a Z-shaped graphene nanoribbon junction. Applied Physics Letters, 2008, 92, .	3.3	55
106	Average density of states in disordered graphene systems. Physical Review B, 2008, 77, .	3.2	54
107	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
108	ELECTRONIC AND STERIC MECHANISMS IN MONO- AND DOUBLE-FLUORINATION OF Cs-C60Cl6. Modern Physics Letters B, 2008, 22, 2727-2738.	1.9	3

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109	Chiral selective tunneling induced negative differential resistance in zigzag graphene nanoribbon: A theoretical study. Applied Physics Letters, 2008, 92, .	3.3	93
110	Quantum Dot Based on Z-shaped Graphene Nanoribbon: First-principles Study. Chinese Journal of Chemical Physics, 2007, 20, 489-494.	1.3	8
111	Switching mechanism of photochromic diarylethene derivatives molecular junctions. Journal of Chemical Physics, 2007, 127, 094705.	3.0	44
112	Z-shaped graphene nanoribbon quantum dot device. Applied Physics Letters, 2007, 91, .	3.3	109
113	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
114	Tuning the electronic structure of graphene nanoribbons through chemical edge modification: A theoretical study. Physical Review B, 2007, 75, .	3.2	156
115	Electronic structure of bilayer graphene: A real-space Greenâ€™s function study. Physical Review B, 2007, 75, .	3.2	35
116	First-principles study ofNi2P(0001) surfaces. Physical Review B, 2006, 74, .	3.2	52
117	Electronic and magnetic properties of V-doped anataseTiO2from first principles. Physical Review B, 2006, 74, .	3.2	80
118	Single quintuple bond [PhCrCrPh] molecule as a possible molecular switch. Journal of Chemical Physics, 2006, 125, 184713.	3.0	19
119	TRANSPORT PROPERTY OF TWO ISOELECTRONIC MOLECULES. International Journal of Nanoscience, 2006, 05, 841-846.	0.7	2
120	Electronic transport property of 4,4â€²-bipyridine molecular junction. Ultramicroscopy, 2005, 105, 293-298.	1.9	15
121	Controlling the Kondo Effect of an Adsorbed Magnetic Ion Through Its Chemical Bonding. Science, 2005, 309, 1542-1544.	12.6	594
122	Nonequilibrium electronic transport of 4,4â€²-bipyridine molecular junction. Journal of Chemical Physics, 2005, 123, 184712.	3.0	59
123	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
124	A theoretical investigation of GenSn (n=1â€“4) clusters. Computational and Theoretical Chemistry, 2003, 624, 257-265.	1.5	14
125	Low-Temperature Orientationally Ordered Structures of Two-Dimensional C60. Journal of the American Chemical Society, 2003, 125, 169-172.	13.7	53
126	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

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127	Unveiling Metal-Cage Hybrid States in a Single Endohedral Metallofullerene. Physical Review Letters, 2003, 91, 185504.	7.8	61
128	First-principles simulation of scanning tunneling microscopy images of individual molecules in alkanethiol self-assembled monolayers on Au(111). , 2003, , .		1
129	A first-principles study of acetylene and its evolution products on Cu(001). Journal of Chemical Physics, 2002, 116, 3104-3108.	3.0	8
130	Topology of two-dimensional C60 domains. Nature, 2001, 409, 304-305.	27.8	101
131	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
132	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
133	Houet al.Reply:. Physical Review Letters, 2000, 85, 2654-2654.	7.8	7
134	Electronic structure of Ti2AlNb (O phase). Journal of Physics Condensed Matter, 1999, 11, 6179-6186.	1.8	10
135	Identifying Molecular Orientation of IndividualC60on aSi(111)â˜'(7Ã—7)Surface. Physical Review Letters, 1999, 83, 3001-3004.	7.8	135
136	Scanning tunneling spectroscopy of individual C60 molecules adsorbed on Si(111)-7Ã—7 surface. Surface Science, 1999, 442, L1024-L1028.	1.9	42
137	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