

Liang Xu

List of Publications by Year in descending order

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30
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49
g-index

100
all docs

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docs citations

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times ranked

2984
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#	ARTICLE	IF	CITATIONS
1	Insights into Enhanced Visible-Light Photocatalytic Hydrogen Evolution of g-C ₃ N ₄ and Highly Reduced Graphene Oxide Composite: The Role of Oxygen. <i>Chemistry of Materials</i> , 2015, 27, 1612-1621.	6.7	252
2	Microstructure evolution and texture tailoring of reduced graphene oxide reinforced Zn scaffold. <i>Bioactive Materials</i> , 2021, 6, 1230-1241.	15.6	132
3	Direct Attack and Indirect Transfer Mechanisms Dominated by Reactive Oxygen Species for Photocatalytic H ₂ O ₂ Production on g-C ₃ N ₄ Possessing Nitrogen Vacancies. <i>ACS Catalysis</i> , 2021, 11, 11440-11450.	11.2	132
4	Two-Dimensional MoS ₂ -Graphene-Based Multilayer van der Waals Heterostructures: Enhanced Charge Transfer and Optical Absorption, and Electric-Field Tunable Dirac Point and Band Gap. <i>Chemistry of Materials</i> , 2017, 29, 5504-5512.	6.7	131
5	Quasi-solid-state Zn-air batteries with an atomically dispersed cobalt electrocatalyst and organohydrogel electrolyte. <i>Nature Communications</i> , 2022, 13, .	12.8	127
6	NiCoP nanoleaves array for electrocatalytic alkaline H ₂ evolution and overall water splitting. <i>Journal of Energy Chemistry</i> , 2020, 50, 395-401.	12.9	103
7	Carbon nanotube-encapsulated cobalt for oxygen reduction: integration of space confinement and N-doping. <i>Chemical Communications</i> , 2019, 55, 14801-14804.	4.1	85
8	Mechanism of Superior Visible-Light Photocatalytic Activity and Stability of Hybrid Ag ₃ PO ₄ /Graphene Nanocomposite. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12972-12979.	3.1	78
9	Interfacial Interactions of Semiconductor with Graphene and Reduced Graphene Oxide: CeO ₂ as a Case Study. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 20350-20357.	8.0	71
10	SiC/MoS ₂ layered heterostructures: Promising photocatalysts revealed by a first-principles study. <i>Materials Chemistry and Physics</i> , 2018, 216, 64-71.	4.0	63
11	Electron accumulation enables Bi efficient CO ₂ reduction for formate production to boost clean Zn-CO ₂ batteries. <i>Nano Energy</i> , 2022, 92, 106780.	16.0	54
12	Defect-engineered 2D/2D hBN/g-C ₃ N ₄ Z-scheme heterojunctions with full visible-light absorption: Efficient metal-free photocatalysts for hydrogen evolution. <i>Applied Surface Science</i> , 2021, 547, 149207.	6.1	51
13	Magnetic properties in Nitrogen-doped SnO ₂ from first-principle study. <i>Solid State Communications</i> , 2009, 149, 1304-1307.	1.9	50
14	Reveal Brønsted-Evans-Polanyi relation and attack mechanisms of reactive oxygen species for photocatalytic H ₂ O ₂ production. <i>Applied Catalysis B: Environmental</i> , 2022, 301, 120757.	20.2	50
15	A novel design of SiH/CeO ₂ (111) van der Waals type-II heterojunction for water splitting. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2812-2818.	2.8	49
16	Boosting the photocatalytic hydrogen evolution performance of monolayer C ₂ N coupled with MoSi ₂ N ₄ : density-functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8318-8325.	2.8	49
17	Two-dimensional H-TiO ₂ /MoS ₂ (WS ₂) van der Waals heterostructures for visible-light photocatalysis and energy conversion. <i>Applied Surface Science</i> , 2020, 504, 144425.	6.1	48
18	Phosphating-induced charge transfer on CoO/CoP interface for alkaline H ₂ evolution. <i>Chinese Chemical Letters</i> , 2021, 32, 3355-3358.	9.0	45

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19	Insights into enhanced visible-light photocatalytic activity of CeO ₂ doped with nonmetal impurity from the first principles. <i>Materials Science in Semiconductor Processing</i> , 2016, 41, 200-208.	4.0	44
20	Rational designed Co@N-doped carbon catalyst for high-efficient H ₂ S selective oxidation by regulating electronic structures. <i>Chemical Engineering Journal</i> , 2020, 401, 126038.	12.7	43
21	Modulating the properties of multi-functional molecular devices consisting of zigzag gallium nitride nanoribbons by different magnetic orderings: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5726-5733.	2.8	42
22	Z-scheme systems of ASi ₂ N ₄ (A=Mo or W) for photocatalytic water splitting and nanogenerators. <i>Tungsten</i> , 2022, 4, 52-59.	4.8	41
23	Origin of enhanced visible-light photocatalytic activity of transition-metal (Fe, Cr and Co)-doped CeO ₂ : effect of 3d orbital splitting. <i>Applied Physics A: Materials Science and Processing</i> , 2017, 123, 1.	2.3	37
24	Rationally designed 2D/2D SiC/g-C ₃ N ₄ photocatalysts for hydrogen production. <i>Catalysis Science and Technology</i> , 2019, 9, 3896-3906.	4.1	35
25	Facile shape-controllable synthesis of Ag ₃ PO ₄ photocatalysts. <i>Materials Letters</i> , 2014, 133, 139-142.	2.6	33
26	Band engineering of ZnS by codoping for visible-light photocatalysis. <i>Applied Physics A: Materials Science and Processing</i> , 2014, 116, 741-750.	2.3	32
27	Electronic Structures and Photocatalytic Responses of SrTiO ₃ (100) Surface Interfaced with Graphene, Reduced Graphene Oxide, and Graphane: Surface Termination Effect. <i>Journal of Physical Chemistry C</i> , 2015, 119, 19095-19104.	3.1	32
28	A simple strategy to construct cobalt oxide-based high-efficiency electrocatalysts with oxygen vacancies and heterojunctions. <i>Electrochimica Acta</i> , 2019, 326, 134979.	5.2	32
29	High-performance bifunctional Fe-doped molybdenum oxide-based electrocatalysts with in situ grown epitaxial heterojunctions for overall water splitting. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 24828-24839.	7.1	32
30	Two-dimensional hexagonal chromium chalcogenides with large vertical piezoelectricity, high-temperature ferromagnetism, and high magnetic anisotropy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14503-14513.	2.8	32
31	Insights into enhanced visible-light photocatalytic activity of C ₆₀ modified g-C ₃ N ₄ hybrids: the role of nitrogen. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 33094-33102.	2.8	31
32	Insight into enhanced visible-light photocatalytic activity of SWCNTs/g-C ₃ N ₄ nanocomposites from first principles. <i>Applied Surface Science</i> , 2020, 530, 147181.	6.1	30
33	Electric-field-induced widely tunable direct and indirect band gaps in hBN/MoS ₂ van der Waals heterostructures. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4426-4434.	5.5	29
34	Electronic properties and photoactivity of monolayer MoS ₂ /fullerene van der Waals heterostructures. <i>RSC Advances</i> , 2016, 6, 43228-43236.	3.6	28
35	Ferromagnetic and metallic properties of the semihydrogenated GaN sheet. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1442-1445.	1.5	27
36	First-principles study of magnetic properties in Ag-doped SnO ₂ . <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 1961-1966.	1.5	26

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37	Spin-dependent transport properties of a chromium porphyrin-based molecular embedded between two graphene nanoribbon electrodes. RSC Advances, 2014, 4, 60376-60381.	3.6	26
38	Band structure engineering of monolayer MoS ₂ : a charge compensated codoping strategy. RSC Advances, 2015, 5, 7944-7952.	3.6	26
39	Tuning near-gap electronic structure, interface charge transfer and visible light response of hybrid doped graphene and Ag ₃ PO ₄ composite: Dopant effects. Scientific Reports, 2016, 6, 22267.	3.3	24
40	Two-dimensional PtSe ₂ /hBN vdW heterojunction as photoelectrocatalyst for the solar-driven oxygen evolution reaction: A first principles study. Applied Surface Science, 2021, 570, 151207.	6.1	24
41	Electronic structures and transport properties of low-dimensional GaN nanoderivatives: A first-principles study. Applied Surface Science, 2021, 561, 150038.	6.1	23
42	Ga-doped Pd/CeO ₂ model catalysts for CO oxidation reactivity: A density functional theory study. Applied Surface Science, 2022, 575, 151655.	6.1	23
43	Enhanced photocatalytic performance of an Ag ₃ PO ₄ photocatalyst via fullerene modification: first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 2878-2886.	2.8	22
44	Direction and strain controlled anisotropic transport behaviors of 2D GeSe-phosphorene vdW heterojunctions. Nanotechnology, 2019, 30, 445703.	2.6	22
45	2D layered SiC/C ₂ N van der Waals type-II heterostructure: a visible-light-driven photocatalyst for water splitting. New Journal of Chemistry, 2020, 44, 15439-15445.	2.8	21
46	Layer-dependent photocatalysts of GaN/SiC-based multilayer van der Waals heterojunctions for hydrogen evolution. Catalysis Science and Technology, 2021, 11, 3059-3069.	4.1	21
47	Hybrid TiO ₂ /graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. Catalysis Science and Technology, 2017, 7, 1423-1432.	4.1	20
48	A novel photocatalyst CeF ₃ : facile fabrication and photocatalytic performance. RSC Advances, 2015, 5, 95171-95177.	3.6	19
49	Type-II CeO ₂ (111)/hBN vdW heterojunction for enhanced photocatalytic hydrogen evolution: A first principles study. International Journal of Hydrogen Energy, 2021, 46, 25060-25069.	7.1	19
50	GaN/Surface-modified graphitic carbon nitride heterojunction: Promising photocatalytic hydrogen evolution materials. International Journal of Hydrogen Energy, 2022, 47, 7202-7213.	7.1	18
51	First-principles study of magnetic properties in Co-doped BiFeO ₃ . Physica B: Condensed Matter, 2015, 457, 1-4.	2.7	17
52	Wrapping effect of secondary phases on the grains: increased corrosion resistance of Mg-Al alloys. Virtual and Physical Prototyping, 2018, 13, 292-300.	10.4	17
53	Multifunctional silicene/CeO ₂ heterojunctions: Desirable electronic material and promising water-splitting photocatalyst. Chinese Chemical Letters, 2022, 33, 3947-3950.	9.0	17
54	Electronic structure and magnetic interactions in Ni-doped $\hat{\Gamma}$ -Ga ₂ O ₃ from first-principles calculations. Scripta Materialia, 2009, 61, 477-480.	5.2	16

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55	Theoretical insight into the electronic and photocatalytic properties of Cu ₂ O from a hybrid density functional theory. <i>Materials Science in Semiconductor Processing</i> , 2014, 23, 34-41.	4.0	16
56	Native vacancy defects in bismuth sulfide. <i>International Journal of Modern Physics B</i> , 2014, 28, 1450150.	2.0	15
57	Dual-Band Plasmonic Perfect Absorber Based on the Hybrid Halide Perovskite in the Communication Regime. <i>Coatings</i> , 2021, 11, 67.	2.6	14
58	Ab initio studies of half-metallic ferromagnetism in carbon-doped. <i>Solid State Communications</i> , 2010, 150, 923-927.	1.9	13
59	Ferromagnetism in zigzag GaN nanoribbons with tunable half-metallic gap. <i>Computational Materials Science</i> , 2016, 117, 300-305.	3.0	13
60	Elasticity, piezoelectricity, and mobility in two-dimensional BiTeI from a first-principles study. <i>Journal Physics D: Applied Physics</i> , 2020, 53, 245301.	2.8	13
61	Semiconductor to metal transition by tuning the location of N ₂ AA in armchair graphene nanoribbons. <i>Journal of Applied Physics</i> , 2014, 115, 053707.	2.5	12
62	Realistic-contact-induced enhancement of rectifying in carbon-nanotube/graphene-nanoribbon junctions. <i>Applied Physics Letters</i> , 2014, 104, 103107.	3.3	12
63	Electronic structure and magnetic properties in Nitrogen-doped from density functional calculations. <i>Solid State Communications</i> , 2010, 150, 852-856.	1.9	11
64	Rectification induced in N ₂ AA-doped armchair graphene nanoribbon device. <i>Journal of Applied Physics</i> , 2014, 116, .	2.5	11
65	Characteristics of electronic and spin-independent linear conductance in conjugated aromatic polymer based molecular device. <i>Organic Electronics</i> , 2019, 65, 49-55.	2.6	11
66	Ferromagnetic coupling in Mg-doped passivated AlN nanowires: A first-principles study. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 185-189.	1.5	10
67	A broadband and polarization-insensitive perfect absorber based on a van der Waals material in the mid-infrared regime. <i>Results in Physics</i> , 2019, 15, 102687.	4.1	10
68	Multiple Heterojunction System of Boron Nitride-Graphene/Black Phosphorene as Highly Efficient Solar Cell. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100169.	2.8	10
69	Graphene-enabled reconfigurable terahertz wavefront modulator based on complete Fermi level modulated phase. <i>New Journal of Physics</i> , 2020, 22, 063054.	2.9	10
70	Band-Gap Widening of Nitrogen-Doped Cu ₂ O: New Insights from First-Principles Calculations. <i>Science of Advanced Materials</i> , 2014, 6, 1221-1227.	0.7	10
71	A comparative study on magnetism in Zn-doped AlN and GaN from first-principles. <i>Journal of Applied Physics</i> , 2014, 116, .	2.5	9
72	Origin of photocatalytic activity of nitrogen-doped germanium dioxide under visible light from first principles. <i>Materials Science in Semiconductor Processing</i> , 2015, 31, 517-524.	4.0	8

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73	Dual functions of 2D WS ₂ and MoS ₂ â€“WS ₂ monolayers coupled with a Ag ₃ PO ₄ photocatalyst. Semiconductor Science and Technology, 2016, 31, 095013.	2.0	8
74	Dual-band perfect absorber based on a graphene/hexagonal boron nitride van der Waals hybrid structure. Journal Physics D: Applied Physics, 0, , .	2.8	8
75	Magnetic properties in nitrogen-doped CeO ₂ from first-principles calculations. Physica B: Condensed Matter, 2010, 405, 4858-4862.	2.7	7
76	Electronic and magnetism properties of half-bare zigzag silicon carbon nanoribbons from hybrid density functional calculations. Solid State Communications, 2013, 158, 25-28.	1.9	7
77	Stable Metallicity of Low Dimensional WCrC Derivatives: A Firstâ€“Principles Study. Advanced Theory and Simulations, 2021, 4, 2100036.	2.8	7
78	Constitutive Model Parameter Identification for 6063 Aluminum Alloy Using Inverse Analysis Method for Extrusion Applications. Journal of Materials Engineering and Performance, 2021, 30, 7449-7460.	2.5	7
79	Spin and band-gap engineering in zigzag graphene nanoribbons with methylene group. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 63, 259-263.	2.7	6
80	Mechanism of enhanced photocatalytic activities on tungsten trioxide doped with sulfur: Dopant-type effects. Modern Physics Letters B, 2016, 30, 1650340.	1.9	6
81	High-performance spin rectification in gallium nitride-based molecular junctions with asymmetric edge passivation. Journal of Applied Physics, 2018, 124, .	2.5	6
82	The effects of heteroatoms-doping on the stability, electronic and magnetic properties of CH ₃ NH ₃ PbI ₃ perovskite. Surfaces and Interfaces, 2021, 24, 101027.	3.0	6
83	The effects of vacancy and heteroatoms-doping on the stability, electronic and magnetic properties of blue phosphorene. Nanotechnology, 2021, 32, 135702.	2.6	5
84	Magnetic properties in a IIIA-nitride monolayer doped with Ag: A density functional theory investigation. Results in Physics, 2022, 35, 105396.	4.1	5
85	Modulation of electronic structure properties of C/B/Al-doped armchair GaN nanoribbons. Molecular Physics, 2020, 118, e1656833.	1.7	4
86	Carbon phosphide nanosheets and nanoribbons: insights on modulating their electronic properties by first principles calculations. Physical Chemistry Chemical Physics, 2020, 22, 22520-22528.	2.8	4
87	High performance Sr ₄ Al ₁₄ O ₂₅ :Mn ⁴⁺ phosphor: structure calculation and optical properties. Journal of Materials Chemistry C, 2022, 10, 7909-7916.	5.5	4
88	Fantastic parity effects on the electronic and magnetic properties of zigzag graphene nanoribbons with side-attached trans-polyacetylene. Europhysics Letters, 2015, 111, 17006.	2.0	3
89	Plasmon Resonances in a Periodic Square Coaxial Hole Array in a Graphene Sheet. Plasmonics, 2016, 11, 1129-1137.	3.4	3
90	Spin-filtering and giant magnetoresistance effects in polyacetylene-based molecular devices. Journal of Applied Physics, 2017, 122, 035103.	2.5	3

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91	Modulation of Electronic Behaviors of InSe Nanosheet and Nanoribbons: The First-Principles Study. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900099.	2.8	3
92	Waveguide-Coupled Surface Plasmon Resonance Sensor for Both Liquid and Gas Detections. <i>Plasmonics</i> , 2020, 15, 1123-1131.	3.4	3
93	Half-metallic ferromagnetism in Fe-chain-embedded zigzag boron-nitride nanoribbons with line defect. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 74, 431-437.	2.7	2
94	First-principles calculations of half-metallic ferromagnetism in zigzag boron-nitride nanoribbons jointed with a single Fe-chain. <i>Journal of Semiconductors</i> , 2015, 36, 082003.	3.7	2
95	Enhanced ferromagnetism by adding electrons in triple-decker Gd-phthalocyanine. <i>Physica Scripta</i> , 2013, 87, 045701.	2.5	1
96	Light transmission through a one-dimensional metallic grating covered by a reduced cytochrome c molecule layer. <i>International Journal of Modern Physics B</i> , 2016, 30, 1650088.	2.0	1
97	Surface dangling bonds dependent magnetic properties in Mn-doped GaAs nanowires. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126815.	2.1	1
98	Removal of Elemental Mercury from Simulated Flue Gas by a Copper-Based ZSM-5 Molecular Sieve. <i>Coatings</i> , 2022, 12, 772.	2.6	1
99	The effects of Co/Ni-vacancy complex defects on the electronic and transport properties of armchair silicene nanoribbon. <i>Pramana - Journal of Physics</i> , 2022, 96, 1.	1.8	0