

Liang Xu

List of Publications by Year in descending order

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99
papers

2,872
citations

159585

30
h-index

197818

49
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all docs

100
docs citations

100
times ranked

2984
citing authors

#	ARTICLE	IF	CITATIONS
1	Z-scheme systems of AsI_2N_4 ($\text{A}=\text{Mo}$ or W) for photocatalytic water splitting and nanogenerators. <i>Tungsten</i> , 2022, 4, 52-59.	4.8	41
2	Reveal Brønsted-Evans-Polanyi relation and attack mechanisms of reactive oxygen species for photocatalytic H_2O_2 production. <i>Applied Catalysis B: Environmental</i> , 2022, 301, 120757.	20.2	50
3	Ga-doped Pd/CeO ₂ model catalysts for CO oxidation reactivity: A density functional theory study. <i>Applied Surface Science</i> , 2022, 575, 151655.	6.1	23
4	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
5	Multifunctional silicene/CeO ₂ heterojunctions: Desirable electronic material and promising water-splitting photocatalyst. <i>Chinese Chemical Letters</i> , 2022, 33, 3947-3950.	9.0	17
6	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
7	GaN/Surface-modified graphitic carbon nitride heterojunction: Promising photocatalytic hydrogen evolution materials. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 7202-7213.	7.1	18
8	Magnetic properties in a IIIA-nitride monolayer doped with Ag: A density functional theory investigation. <i>Results in Physics</i> , 2022, 35, 105396.	4.1	5
9	High performance Sr ₄ Al ₁₄ O ₂₅ :Mn ⁴⁺ phosphor: structure calculation and optical properties. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7909-7916.	5.5	4
10	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
11	Quasi-solid-state Zn-air batteries with an atomically dispersed cobalt electrocatalyst and organohydrogel electrolyte. <i>Nature Communications</i> , 2022, 13, .	12.8	127
12	Microstructure evolution and texture tailoring of reduced graphene oxide reinforced Zn scaffold. <i>Bioactive Materials</i> , 2021, 6, 1230-1241.	15.6	132
13	Layer-dependent photocatalysts of GaN/SiC-based multilayer van der Waals heterojunctions for hydrogen evolution. <i>Catalysis Science and Technology</i> , 2021, 11, 3059-3069.	4.1	21
14	Dual-Band Plasmonic Perfect Absorber Based on the Hybrid Halide Perovskite in the Communication Regime. <i>Coatings</i> , 2021, 11, 67.	2.6	14
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	Stable Metallicity of Low Dimensional WC ₂ Derivatives: A First-Principles Study. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100036.	2.8	7
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	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
20	The effects of heteroatoms-doping on the stability, electronic and magnetic properties of CH ₃ NH ₃ PbI ₃ perovskite. <i>Surfaces and Interfaces</i> , 2021, 24, 101027.	3.0	6
21	Constitutive Model Parameter Identification for 6063 Aluminum Alloy Using Inverse Analysis Method for Extrusion Applications. <i>Journal of Materials Engineering and Performance</i> , 2021, 30, 7449-7460.	2.5	7
22	Type-II CeO ₂ (111)/hBN vdW heterojunction for enhanced photocatalytic hydrogen evolution: A first principles study. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 25060-25069.	7.1	19
23	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
24	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
25	Electronic structures and transport properties of low-dimensional GaN nanoderivatives: A first-principles study. <i>Applied Surface Science</i> , 2021, 561, 150038.	6.1	23
26	Two-dimensional PtSe ₂ /hBN vdW heterojunction as photoelectrocatalyst for the solar-driven oxygen evolution reaction: A first principles study. <i>Applied Surface Science</i> , 2021, 570, 151207.	6.1	24
27	The effects of vacancy and heteroatoms-doping on the stability, electronic and magnetic properties of blue phosphorene. <i>Nanotechnology</i> , 2021, 32, 135702.	2.6	5
28	Modulation of electronic structure properties of C/B/Al-doped armchair GaN nanoribbons. <i>Molecular Physics</i> , 2020, 118, e1656833.	1.7	4
29	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
30	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
31	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
32	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
33	2D layered SiC/C ₂ N van der Waals type-II heterostructure: a visible-light-driven photocatalyst for water splitting. <i>New Journal of Chemistry</i> , 2020, 44, 15439-15445.	2.8	21
34	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
35	Carbon phosphide nanosheets and nanoribbons: insights on modulating their electronic properties by first principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22520-22528.	2.8	4
36	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

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37	Elasticity, piezoelectricity, and mobility in two-dimensional BiTeI from a first-principles study. Journal Physics D: Applied Physics, 2020, 53, 245301.	2.8	13
38	Waveguide-Coupled Surface Plasmon Resonance Sensor for Both Liquid and Gas Detections. Plasmonics, 2020, 15, 1123-1131.	3.4	3
39	NiCoP nanoleaves array for electrocatalytic alkaline H ₂ evolution and overall water splitting. Journal of Energy Chemistry, 2020, 50, 395-401.	12.9	103
40	Graphene-enabled reconfigurable terahertz wavefront modulator based on complete Fermi level modulated phase. New Journal of Physics, 2020, 22, 063054.	2.9	10
41	Direction and strain controlled anisotropic transport behaviors of 2D GeSe-phosphorene vdW heterojunctions. Nanotechnology, 2019, 30, 445703.	2.6	22
42	Modulation of Electronic Behaviors of InSe Nanosheet and Nanoribbons: The First-Principles Study. Advanced Theory and Simulations, 2019, 2, 1900099.	2.8	3
43	A broadband and polarization-insensitive perfect absorber based on a van der Waals material in the mid-infrared regime. Results in Physics, 2019, 15, 102687.	4.1	10
44	A simple strategy to construct cobalt oxide-based high-efficiency electrocatalysts with oxygen vacancies and heterojunctions. Electrochimica Acta, 2019, 326, 134979.	5.2	32
45	Rationally designed 2D/2D SiC/g-C ₃ N ₄ photocatalysts for hydrogen production. Catalysis Science and Technology, 2019, 9, 3896-3906.	4.1	35
46	Carbon nanotube-encapsulated cobalt for oxygen reduction: integration of space confinement and N-doping. Chemical Communications, 2019, 55, 14801-14804.	4.1	85
47	Characteristics of electronic and spin-independent linear conductance in conjugated aromatic polymer based molecular device. Organic Electronics, 2019, 65, 49-55.	2.6	11
48	Modulating the properties of multi-functional molecular devices consisting of zigzag gallium nitride nanoribbons by different magnetic orderings: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 5726-5733.	2.8	42
49	High-performance spin rectification in gallium nitride-based molecular junctions with asymmetric edge passivation. Journal of Applied Physics, 2018, 124, .	2.5	6
50	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
51	SiC/MoS ₂ layered heterostructures: Promising photocatalysts revealed by a first-principles study. Materials Chemistry and Physics, 2018, 216, 64-71.	4.0	63
52	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
53	Origin of enhanced visible-light photocatalytic activity of transition-metal (Fe, Cr and Co)-doped CeO ₂ : effect of 3d orbital splitting. Applied Physics A: Materials Science and Processing, 2017, 123, 1.	2.3	37
54	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. Chemistry of Materials, 2017, 29, 5504-5512.	6.7	131

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55	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
56	Spin-filtering and giant magnetoresistance effects in polyacetylene-based molecular devices. <i>Journal of Applied Physics</i> , 2017, 122, 035103.	2.5	3
57	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
58	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
59	Electronic properties and photoactivity of monolayer MoS ₂ /fullerene van der Waals heterostructures. <i>RSC Advances</i> , 2016, 6, 43228-43236.	3.6	28
60	Mechanism of enhanced photocatalytic activities on tungsten trioxide doped with sulfur: Dopant-type effects. <i>Modern Physics Letters B</i> , 2016, 30, 1650340.	1.9	6
61	Dual functions of 2D WS ₂ and MoS ₂ WS ₂ monolayers coupled with a Ag ₃ PO ₄ photocatalyst. <i>Semiconductor Science and Technology</i> , 2016, 31, 095013.	2.0	8
62	Tuning near-gap electronic structure, interface charge transfer and visible light response of hybrid doped graphene and Ag ₃ PO ₄ composite: Dopant effects. <i>Scientific Reports</i> , 2016, 6, 22267.	3.3	24
63	Enhanced photocatalytic performance of an Ag ₃ PO ₄ photocatalyst via fullerene modification: first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2878-2886.	2.8	22
64	Ferromagnetism in zigzag GaN nanoribbons with tunable half-metallic gap. <i>Computational Materials Science</i> , 2016, 117, 300-305.	3.0	13
65	Plasmon Resonances in a Periodic Square Coaxial Hole Array in a Graphene Sheet. <i>Plasmonics</i> , 2016, 11, 1129-1137.	3.4	3
66	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
67	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
68	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
69	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
70	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
71	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
72	A novel photocatalyst CeF ₃ : facile fabrication and photocatalytic performance. <i>RSC Advances</i> , 2015, 5, 95171-95177.	3.6	19

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73	Fantastic parity effects on the electronic and magnetic properties of zigzag graphene nanoribbons with side-attached trans-polyacetylene. <i>Europhysics Letters</i> , 2015, 111, 17006.	2.0	3
74	Band structure engineering of monolayer MoS ₂ : a charge compensated codoping strategy. <i>RSC Advances</i> , 2015, 5, 7944-7952.	3.6	26
75	First-principles study of magnetic properties in Co-doped BiFeO ₃ . <i>Physica B: Condensed Matter</i> , 2015, 457, 1-4.	2.7	17
76	Rectification induced in N ₂ AA-doped armchair graphene nanoribbon device. <i>Journal of Applied Physics</i> , 2014, 116, .	2.5	11
77	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
78	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
79	Spin-dependent transport properties of a chromium porphyrin-based molecular embedded between two graphene nanoribbon electrodes. <i>RSC Advances</i> , 2014, 4, 60376-60381.	3.6	26
80	Realistic-contact-induced enhancement of rectifying in carbon-nanotube/graphene-nanoribbon junctions. <i>Applied Physics Letters</i> , 2014, 104, 103107.	3.3	12
81	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
82	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
83	Spin and band-gap engineering in zigzag graphene nanoribbons with methylene group. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014, 63, 259-263.	2.7	6
84	Native vacancy defects in bismuth sulfide. <i>International Journal of Modern Physics B</i> , 2014, 28, 1450150.	2.0	15
85	Facile shape-controllable synthesis of Ag ₃ PO ₄ photocatalysts. <i>Materials Letters</i> , 2014, 133, 139-142.	2.6	33
86	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
87	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
88	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
89	Electronic and magnetism properties of half-bare zigzag silicon carbon nanoribbons from hybrid density functional calculations. <i>Solid State Communications</i> , 2013, 158, 25-28.	1.9	7
90	Enhanced ferromagnetism by adding electrons in triple-decker Gd-phthalocyanine. <i>Physica Scripta</i> , 2013, 87, 045701.	2.5	1

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91	Ferromagnetic coupling in Mg-doped passivated AlN nanowires: A first-principles study. Physica Status Solidi (B): Basic Research, 2012, 249, 185-189.	1.5	10
92	Ferromagnetic and metallic properties of the semihydrogenated GaN sheet. Physica Status Solidi (B): Basic Research, 2011, 248, 1442-1445.	1.5	27
93	First-principles study of magnetic properties in Ag-doped SnO ₂ . Physica Status Solidi (B): Basic Research, 2011, 248, 1961-1966.	1.5	26
94	Magnetic properties in nitrogen-doped CeO ₂ from first-principles calculations. Physica B: Condensed Matter, 2010, 405, 4858-4862.	2.7	7
95	Electronic structure and magnetic properties in Nitrogen-doped from density functional calculations. Solid State Communications, 2010, 150, 852-856.	1.9	11
96	Ab initio studies of half-metallic ferromagnetism in carbon-doped. Solid State Communications, 2010, 150, 923-927.	1.9	13
97	Electronic structure and magnetic interactions in Ni-doped $\hat{\Gamma}^2$ -Ga ₂ O ₃ from first-principles calculations. Scripta Materialia, 2009, 61, 477-480.	5.2	16
98	Magnetic properties in Nitrogen-doped SnO ₂ from first-principle study. Solid State Communications, 2009, 149, 1304-1307.	1.9	50
99	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