

Xingxing Li

List of Publications by Year in descending order

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72
papers

4,738
citations

156536

32
h-index

111975

67
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72
all docs

72
docs citations

72
times ranked

5729
citing authors

#	ARTICLE	IF	CITATIONS
1	Real-time observation of the dynamics of an individual rotaxane molecular shuttle using a single-molecule junction. <i>CheM</i> , 2022, 8, 243-252.	5.8	29
2	Enhanced Curie Temperature of Two-Dimensional Cr(II) Aromatic Heterocyclic Metal-Organic Framework Magnets via Strengthened Orbital Hybridization. <i>Nano Letters</i> , 2022, 22, 1573-1579.	4.5	25
3	Single-molecule field effect and conductance switching driven by electric field and proton transfer. <i>Science Advances</i> , 2022, 8, eabm3541.	4.7	22
4	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors. <i>Research</i> , 2022, 2022, 9857631.	2.8	4
5	Promoting Water Activation by Photogenerated Holes in Monolayer C ₂ N. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3332-3337.	2.1	7
6	A review of bipolar magnetic semiconductors from theoretical aspects. <i>Fundamental Research</i> , 2022, 2, 511-521.	1.6	19
7	Bipolar Magnetic Molecules for Spin-Polarized Electric Current in Molecular Junctions. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	9
8	Bipolar Magnetic Molecules for Spin-Polarized Electric Current in Molecular Junctions. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2
9	Two-Dimensional Multifunctional Metal-Organic Framework with Intrinsic Bipolar Magnetic Semiconductivity and Negative Poisson's Ratio. <i>ACS Applied Electronic Materials</i> , 2022, 4, 3198-3204.	2.0	6
10	Efficient interlayer charge release for high-performance layered thermoelectrics. <i>National Science Review</i> , 2021, 8, nwa085.	4.6	15
11	Strain-Stabilized Metastable Face-Centered Tetragonal Gold Overlayer for Efficient CO ₂ Electroreduction. <i>Nano Letters</i> , 2021, 21, 1003-1010.	4.5	32
12	CrSbS ₃ monolayer: a potential phase transition ferromagnetic semiconductor. <i>Nanoscale</i> , 2021, 13, 14067-14072.	2.8	5
13	A single-molecule electrical approach for amino acid detection and chirality recognition. <i>Science Advances</i> , 2021, 7, .	4.7	43
14	Orbital Design of Two-Dimensional Transition-Metal Peroxide Kagome Crystals with Anionogenic Dirac Half-Metallicity. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3528-3534.	2.1	7
15	Thickness Dependent Magnetic Transition in Few Layer 1T Phase CrTe ₂ . <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6847-6851.	2.1	19
16	Unveiling the full reaction path of the Suzuki-Miyaura cross-coupling in a single-molecule junction. <i>Nature Nanotechnology</i> , 2021, 16, 1214-1223.	15.6	46
17	A rationally designed two-dimensional MoSe ₂ /TiCO ₂ heterojunction for photocatalytic overall water splitting: simultaneously suppressing electron-hole recombination and photocorrosion. <i>Chemical Science</i> , 2021, 12, 2863-2869.	3.7	82
18	Two-dimensional bipolar magnetic semiconductors with high Curie-temperature and electrically controllable spin polarization realized in exfoliated Cr(pyrazine) ₂ monolayers. <i>Science China Chemistry</i> , 2021, 64, 2212-2217.	4.2	25

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19	Designing Two-Dimensional Versatile Room-Temperature Ferromagnets via Assembling Large-Scale Magnetic Quantum Dots. <i>Nano Letters</i> , 2021, 21, 9816-9823.	4.5	11
20	High Curie Temperature and Intrinsic Ferromagnetic Half-Metallicity in $Mn_{2-x}X_3$ ($X = S, Se, Te$) Nanosheets. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11790-11794.	2.1	14
21	Large Spin-Gap Nodal-Line Half-Metal and High-Temperature Ferromagnetic Semiconductor in $Cr_{2-x}X_3$ ($X=O,S,Se$) Monolayers. <i>Advanced Electronic Materials</i> , 2020, 6, 1900490.	2.6	27
22	Excitons in bent black phosphorus nanoribbons: multiple excitonic funnels. <i>Materials Today Advances</i> , 2020, 7, 100096.	2.5	6
23	Proposed mechanical method for switching the spin transport channel in two-dimensional magnetic metal-magnetic semiconductor van der Waals contacts. <i>Nanoscale Horizons</i> , 2020, 5, 1496-1499.	4.1	5
24	Two-Dimensional Multifunctional Metal-Organic Frameworks with Simultaneous Ferro-/Ferrimagnetism and Vertical Ferroelectricity. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4193-4197.	2.1	30
25	Prediction of $MnSiTe_3$ as an intrinsic layered half-metal. <i>Physical Review B</i> , 2020, 101, .		
26	Halogen modified two-dimensional covalent triazine frameworks as visible-light driven photocatalysts for overall water splitting. <i>Science China Chemistry</i> , 2020, 63, 1134-1141.	4.2	31
27	Atomic-Level Construction of Tensile-Strained PdFe Alloy Surface toward Highly Efficient Oxygen Reduction Electrocatalysis. <i>Nano Letters</i> , 2020, 20, 1403-1409.	4.5	89
28	Are pyridinium ylides radicals?. <i>Chemical Communications</i> , 2020, 56, 11287-11290.	2.2	8
29	Room-Temperature Ferromagnetism in Transition Metal Embedded Borophene Nanosheets. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4417-4421.	2.1	26
30	Significantly Enhanced Charge Separation in Rippled Monolayer Graphitic C_3N_4 . <i>ChemCatChem</i> , 2019, 11, 6252-6257.	1.8	9
31	Computational Design of One-Dimensional Ferromagnetic Semiconductors in Transition Metal Embedded Stannaspherene Nanowires. <i>Chinese Journal of Chemistry</i> , 2019, 37, 1021-1024.	2.6	7
32	Revealing Charge- and Temperature-Dependent Movement Dynamics and Mechanism of Individual Molecular Machines. <i>Small Methods</i> , 2019, 3, 1900464.	4.6	21
33	The Contacts of the Monolayer Semiconductor C_2N with 2D Metal Electrodes. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800161.	1.3	19
34	Unconventional d Hybridization Interaction in PtGa Ultrathin Nanowires Boosts Oxygen Reduction Electrocatalysis. <i>Journal of the American Chemical Society</i> , 2019, 141, 18083-18090.	6.6	216
35	Proposal of a stable B_3S nanosheet as an efficient hydrogen evolution catalyst. <i>Journal of Materials Chemistry A</i> , 2019, 7, 3752-3756.	5.2	41
36	Toward Room-Temperature Magnetic Semiconductors in Two-Dimensional Ferrimagnetic Organometallic Lattices. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2439-2444.	2.1	39

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37	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. <i>Npj 2D Materials and Applications</i> , 2019, 3, .	3.9	25
38	Realizing Two-Dimensional Magnetic Semiconductors with Enhanced Curie Temperature by Antiaromatic Ring Based Organometallic Frameworks. <i>Journal of the American Chemical Society</i> , 2019, 141, 109-112.	6.6	77
39	Construction of direct Z-scheme photocatalysts for overall water splitting using two-dimensional van der Waals heterojunctions of metal dichalcogenides. <i>Journal of Computational Chemistry</i> , 2019, 40, 980-987.	1.5	48
40	Direct observation of single-molecule hydrogen-bond dynamics with single-bond resolution. <i>Nature Communications</i> , 2018, 9, 807.	5.8	78
41	A high performance catalyst for methane conversion to methanol: graphene supported single atom Co. <i>Chemical Communications</i> , 2018, 54, 2284-2287.	2.2	57
42	The roles of buckled geometry and water environment in the excitonic properties of graphitic C ₃ N ₄ . <i>Nanoscale</i> , 2018, 10, 3738-3743.	2.8	17
43	Spatial and thickness dependence of coupling interaction of surface states and influence on transport and optical properties of few-layer Bi ₂ Se ₃ . <i>Journal of Physics Condensed Matter</i> , 2018, 30, 065503.	0.7	3
44	Frontispiz: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. <i>Angewandte Chemie</i> , 2018, 130, .	1.6	0
45	Frontispiece: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. <i>Angewandte Chemie - International Edition</i> , 2018, 57, .	7.2	0
46	Intrinsic Electric Fields in Two-dimensional Materials Boost the Solar-to-Hydrogen Efficiency for Photocatalytic Water Splitting. <i>Nano Letters</i> , 2018, 18, 6312-6317.	4.5	391
47	Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. <i>Angewandte Chemie</i> , 2018, 130, 14222-14227.	1.6	22
48	One-Nanometer-Thick PtNiRh Trimetallic Nanowires with Enhanced Oxygen Reduction Electrocatalysis in Acid Media: Integrating Multiple Advantages into One Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 16159-16167.	6.6	160
49	Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 14026-14031.	7.2	52
50	Low-dimensional half-metallic materials: theoretical simulations and design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1314.	6.2	47
51	Ï-Phosphorene: a new allotrope of phosphorene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 2402-2408.	1.3	65
52	Ï-Phosphorene: a two dimensional material with a highly negative Poisson's ratio. <i>Nanoscale</i> , 2017, 9, 850-855.	2.8	150
53	BP ₅ monolayer with multiferroicity and negative Poisson's ratio: a prediction by global optimization method. <i>2D Materials</i> , 2017, 4, 045020.	2.0	83
54	Two-dimensional multilayer M ₂ CO ₂ (M = Sc, Zr, Hf) as photocatalysts for hydrogen production from water splitting: a first principles study. <i>Journal of Materials Chemistry A</i> , 2017, 5, 24972-24980.	5.2	90

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55	The gâ€C₃N₄/C₂N Nanocomposite: A gâ€C₃N₄-Based Waterâ€Splitting Photocatalyst with Enhanced Energy Efficiency. ChemPhysChem, 2016, 17, 2100-2104.	1.0	118
56	A many-body GWâ€+â€BSE investigation of electronic and optical properties of C2N. Applied Physics Letters, 2016, 109, .	1.5	51
57	First-principles design of spintronics materials. National Science Review, 2016, 3, 365-381.	4.6	344
58	Two-dimensional van der Waals nanocomposites as Z-scheme type photocatalysts for hydrogen production from overall water splitting. Journal of Materials Chemistry A, 2016, 4, 18892-18898.	5.2	108
59	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. Physical Review B, 2015, 92, .	1.1	23
60	Comparative Study on Electronic Structures of Sc and Ti Contacts with Monolayer and Multilayer MoS₂. ACS Applied Materials & Interfaces, 2015, 7, 12981-12987.	4.0	36
61	Electrical control of carriers' spin orientation in the FeVTiSi Heusler alloy. Journal of Materials Chemistry C, 2015, 3, 2563-2567.	2.7	30
62	Single layer of MX₃ (M = Ti, Zr; X = S, Se, Te): a new platform for nano-electronics and optics. Physical Chemistry Chemical Physics, 2015, 17, 18665-18669.	1.3	128
63	SiN-SiC nanofilm: A nano-functional ceramic with bipolar magnetic semiconducting character. Applied Physics Letters, 2014, 104, .	1.5	26
64	Design and Control of the Cryogenic Distillation Process for Purification of Synthetic Natural Gas from Methanation of Coke Oven Gas. Industrial & Engineering Chemistry Research, 2014, 53, 19583-19593.	1.8	23
65	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. Physical Review Letters, 2014, 112, 018301.	2.9	237
66	CrXTe₃ (X = Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors. Journal of Materials Chemistry C, 2014, 2, 7071.	2.7	332
67	Room-Temperature Half-Metallicity in La(Mn,Zn)AsO Alloy via Element Substitutions. Journal of the American Chemical Society, 2014, 136, 5664-5669.	6.6	88
68	Half-Metallicity in MnPSe₃ Exfoliated Nanosheet with Carrier Doping. Journal of the American Chemical Society, 2014, 136, 11065-11069.	6.6	353
69	Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. Physical Chemistry Chemical Physics, 2013, 15, 15793.	1.3	78
70	Control of spin in a La(Mn,Zn)AsO alloy by carrier doping. Journal of Materials Chemistry C, 2013, 1, 7197.	2.7	17
71	Semihydrogenated BN Sheet: A Promising Visible-light Driven Photocatalyst for Water Splitting. Scientific Reports, 2013, 3, 1858.	1.6	127
72	Bipolar magnetic semiconductors: a new class of spintronics materials. Nanoscale, 2012, 4, 5680.	2.8	241