Xingxing Li

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/1350651/publications.pdf

Version: 2024-02-01

72 papers	4,738 citations	136950 32 h-index	98798 67 g-index
72 all docs	72 docs citations	72 times ranked	4924 citing authors

#	Article	IF	Citations
1	Intrinsic Electric Fields in Two-dimensional Materials Boost the Solar-to-Hydrogen Efficiency for Photocatalytic Water Splitting. Nano Letters, 2018, 18, 6312-6317.	9.1	391
2	Half-Metallicity in MnPSe₃ Exfoliated Nanosheet with Carrier Doping. Journal of the American Chemical Society, 2014, 136, 11065-11069.	13.7	353
3	First-principles design of spintronics materials. National Science Review, 2016, 3, 365-381.	9.5	344
4	CrXTe₃(X = Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors. Journal of Materials Chemistry C, 2014, 2, 7071.	5.5	332
5	Bipolar magnetic semiconductors: a new class of spintronics materials. Nanoscale, 2012, 4, 5680.	5.6	241
6	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. Physical Review Letters, 2014, 112, 018301.	7.8	237
7	Unconventional pâ€“d Hybridization Interaction in PtCa Ultrathin Nanowires Boosts Oxygen Reduction Electrocatalysis. Journal of the American Chemical Society, 2019, 141, 18083-18090.	13.7	216
8	One-Nanometer-Thick PtNiRh Trimetallic Nanowires with Enhanced Oxygen Reduction Electrocatalysis in Acid Media: Integrating Multiple Advantages into One Catalyst. Journal of the American Chemical Society, 2018, 140, 16159-16167.	13.7	160
9	Î´-Phosphorene: a two dimensional material with a highly negative Poisson's ratio. Nanoscale, 2017, 9, 850-855.	5.6	150
10	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.	2.8	128
11	Semihydrogenated BN Sheet: A Promising Visible-light Driven Photocatalyst for Water Splitting. Scientific Reports, 2013, 3, 1858.	3.3	127
12	The gâ€C₃N₄/C₂N Nanocomposite: A gâ€C₃N₄â€Based Waterâ€Splitting Photocatalyst with Enhanced Energy Efficiency. ChemPhysChem, 2016, 17, 2100-2104.	2.1	118
13	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.	10.3	108
14	Two-dimensional multilayer M₂CO₂(M = Sc, Zr, Hf) as photocatalysts for hydrogen production from water splitting: a first principles study. Journal of Materials Chemistry A, 2017, 5, 24972-24980.	10.3	90
15	Atomic-Level Construction of Tensile-Strained PdFe Alloy Surface toward Highly Efficient Oxygen Reduction Electrocatalysis. Nano Letters, 2020, 20, 1403-1409.	9.1	89
16	Room-Temperature Half-Metallicity in La(Mn,Zn)AsO Alloy via Element Substitutions. Journal of the American Chemical Society, 2014, 136, 5664-5669.	13.7	88
17	BP ₅ monolayer with multiferroicity and negative Poissonâ€™s ratio: a prediction by global optimization method. 2D Materials, 2017, 4, 045020.	4.4	83
18	A rationally designed two-dimensional MoSe₂/Ti₂CO₂ heterojunction for photocatalytic overall water splitting: simultaneously suppressing electronâ€“hole recombination and photocorrosion. Chemical Science, 2021, 12, 2863-2869.	7.4	82

#	Article	IF	Citations
19	Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. Physical Chemistry Chemical Physics, 2013, 15, 15793.	2.8	78
20	Direct observation of single-molecule hydrogen-bond dynamics with single-bond resolution. Nature Communications, 2018, 9, 807.	12.8	78
21	Realizing Two-Dimensional Magnetic Semiconductors with Enhanced Curie Temperature by Antiaromatic Ring Based Organometallic Frameworks. Journal of the American Chemical Society, 2019, 141, 109-112.	13.7	77
22	Ï^-Phosphorene: a new allotrope of phosphorene. Physical Chemistry Chemical Physics, 2017, 19, 2402-2408.	2.8	65
23	A high performance catalyst for methane conversion to methanol: graphene supported single atom Co. Chemical Communications, 2018, 54, 2284-2287.	4.1	57
24	Tuning Charge Transport in Aromaticâ€Ring Singleâ€Molecule Junctions via Ionicâ€Liquid Gating. Angewandte Chemie - International Edition, 2018, 57, 14026-14031.	13.8	52
25	A many-body GWâ€‰+â€‰BSE investigation of electronic and optical properties of C2N. Applied Physics Letters, 2016, 109, .	3.3	51
26	Construction of direct Zâ€Scheme photocatalysts for overall water splitting using twoâ€dimensional van der waals heterojunctions of metal dichalcogenides. Journal of Computational Chemistry, 2019, 40, 980-987.	3.3	48
27	Lowâ€dimensional halfâ€metallic materials: theoretical simulations and design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1314.	14.6	47
28	Unveiling the full reaction path of the Suzukiâ€“Miyaura cross-coupling in a single-molecule junction. Nature Nanotechnology, 2021, 16, 1214-1223.	31.5	46
29	A single-molecule electrical approach for amino acid detection and chirality recognition. Science Advances, 2021, 7, .	10.3	43
30	Proposal of a stable B₃S nanosheet as an efficient hydrogen evolution catalyst. Journal of Materials Chemistry A, 2019, 7, 3752-3756.	10.3	41
31	Toward Room-Temperature Magnetic Semiconductors in Two-Dimensional Ferrimagnetic Organometallic Lattices. Journal of Physical Chemistry Letters, 2019, 10, 2439-2444.	4.6	39
32	Comparative Study on Electronic Structures of Sc and Ti Contacts with Monolayer and Multilayer MoS₂. ACS Applied Materials & Interfaces, 2015, 7, 12981-12987.	8.0	36
33	Strain-Stabilized Metastable Face-Centered Tetragonal Gold Overlayer for Efficient CO₂ Electroreduction. Nano Letters, 2021, 21, 1003-1010.	9.1	32
34	Halogen modified two-dimensional covalent triazine frameworks as visible-light driven photocatalysts for overall water splitting. Science China Chemistry, 2020, 63, 1134-1141.	8.2	31
35	Electrical control of carriers' spin orientation in the FeVTiSi Heusler alloy. Journal of Materials Chemistry C, 2015, 3, 2563-2567.	5.5	30
36	Two-Dimensional Multifunctional Metalâ€“Organic Frameworks with Simultaneous Ferro-/Ferrimagnetism and Vertical Ferroelectricity. Journal of Physical Chemistry Letters, 2020, 11, 4193-4197.	4.6	30

#	Article	IF	Citations
37	Real-time observation of the dynamics of an individual rotaxane molecular shuttle using a single-molecule junction. CheM, 2022, 8, 243-252.	11.7	29
38	Largeâ€Spinâ€Gap Nodalâ€Line Halfâ€Metal and Highâ€Temperature Ferromagnetic Semiconductor in Cr₂X₃ (X=O,S,Se) Monolayers. Advanced Electronic Materials, 2020, 6, 1900490.	5.1	27
39	SiN-SiC nanofilm: A nano-functional ceramic with bipolar magnetic semiconducting character. Applied Physics Letters, 2014, 104, .	3.3	26
40	Room-Temperature Ferromagnetism in Transition Metal Embedded Borophene Nanosheets. Journal of Physical Chemistry Letters, 2019, 10, 4417-4421.	4.6	26
41	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, .	7.9	25
42	Two-dimensional bipolar magnetic semiconductors with high Curie-temperature and electrically controllable spin polarization realized in exfoliated Cr(pyrazine)2 monolayers. Science China Chemistry, 2021, 64, 2212-2217.	8.2	25
43	Enhanced Curie Temperature of Two-Dimensional Cr(II) Aromatic Heterocyclic Metalâ€“Organic Framework Magnets via Strengthened Orbital Hybridization. Nano Letters, 2022, 22, 1573-1579.	9.1	25
44	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.	3.7	23
45	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. Physical Review B, 2015, 92, .	3.2	23
46	Tuning Charge Transport in Aromaticâ€Ring Singleâ€Molecule Junctions via Ionicâ€Liquid Gating. Angewandte Chemie, 2018, 130, 14222-14227.	2.0	22
47	Single-molecule field effect and conductance switching driven by electric field and proton transfer. Science Advances, 2022, 8, eabm3541.	10.3	22
48	Revealing Chargeâ€and Temperatureâ€Dependent Movement Dynamics and Mechanism of Individual Molecular Machines. Small Methods, 2019, 3, 1900464.	8.6	21
49	The Contacts of the Monolayer Semiconductor C₂N with 2D Metal Electrodes. Advanced Theory and Simulations, 2019, 2, 1800161.	2.8	19
50	Thickness Dependent Magnetic Transition in Few Layer 1T Phase CrTe₂. Journal of Physical Chemistry Letters, 2021, 12, 6847-6851.	4.6	19
51	A review of bipolar magnetic semiconductors from theoretical aspects. Fundamental Research, 2022, 2, 511-521.	3.3	19
52	Control of spin in a La(Mn,Zn)AsO alloy by carrier doping. Journal of Materials Chemistry C, 2013, 1, 7197.	5.5	17
53	The roles of buckled geometry and water environment in the excitonic properties of graphitic C₃N₄. Nanoscale, 2018, 10, 3738-3743.	5.6	17
54	Prediction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnSiTe</mml:mi><mml:mn>3</mml:mn></mml:msub></ as an intrinsic layered half-metal. Physical Review B, 2020, 101, .	3.2	17

#	Article	IF	Citations
55	Efficient interlayer charge release for high-performance layered thermoelectrics. National Science Review, 2021, 8, nwaa085.	9.5	15
56	High Curie Temperature and Intrinsic Ferromagnetic Half-Metallicity in Mn₂X₃ (X = S, Se, Te) Nanosheets. Journal of Physical Chemistry Letters, 2021, 12, 11790-11794.	4.6	14
57	Designing Two-Dimensional Versatile Room-Temperature Ferromagnets via Assembling Large-Scale Magnetic Quantum Dots. Nano Letters, 2021, 21, 9816-9823.	9.1	11
58	Significantly Enhanced Charge Separation in Rippled Monolayer Graphitic C 3 N 4. ChemCatChem, 2019, 11, 6252-6257.	3.7	9
59	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie - International Edition, 2022, 61, .	13.8	9
60	Are pyridinium ylides radicals?. Chemical Communications, 2020, 56, 11287-11290.	4.1	8
61	Computational Design of Oneâ€Dimensional Ferromagnetic Semiconductors in Transition Metal Embedded Stannaspherene Nanowires. Chinese Journal of Chemistry, 2019, 37, 1021-1024.	4.9	7
62	Orbital Design of Two-Dimensional Transition-Metal Peroxide Kagome Crystals with Anionogenic Dirac Half-Metallicity. Journal of Physical Chemistry Letters, 2021, 12, 3528-3534.	4.6	7
63	Promoting Water Activation by Photogenerated Holes in Monolayer C₂N. Journal of Physical Chemistry Letters, 2022, 13, 3332-3337.	4.6	7
64	Excitons in bent black phosphorus nanoribbons: multiple excitonic funnels. Materials Today Advances, 2020, 7, 100096.	5.2	6
65	Two-Dimensional Multifunctional Metalâ€“Organic Framework with Intrinsic Bipolar Magnetic Semiconductivity and Negative Poissonâ€™s Ratio. ACS Applied Electronic Materials, 2022, 4, 3198-3204.	4.3	6
66	Proposed mechanical method for switching the spin transport channel in two-dimensional magnetic metalâ€“magnetic semiconductor van der Waals contacts. Nanoscale Horizons, 2020, 5, 1496-1499.	8.0	5
67	CrSbS₃ monolayer: a potential phase transition ferromagnetic semiconductor. Nanoscale, 2021, 13, 14067-14072.	5.6	5
68	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors. Research, 2022, 2022, 9857631.	5.7	4
69	Spatial and thickness dependence of coupling interaction of surface states and influence on transport and optical properties of few-layer Bi2Se3. Journal of Physics Condensed Matter, 2018, 30, 065503.	1.8	3
70	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie, 2022, 134, .	2.0	2
71	Frontispiz: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. Angewandte Chemie, 2018, 130, .	2.0	0
72	Frontispiece: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. Angewandte Chemie - International Edition, 2018, 57, .	13.8	0