Xingxing Li

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	Enhanced Curie Temperature of Two-Dimensional Cr(II) Aromatic Heterocyclic Metal–Organic Framework Magnets via Strengthened Orbital Hybridization. Nano Letters, 2022, 22, 1573-1579.	9.1	25
3	Single-molecule field effect and conductance switching driven by electric field and proton transfer. Science Advances, 2022, 8, eabm3541.	10.3	22
4	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors. Research, 2022, 2022, 9857631.	5.7	4
5	Promoting Water Activation by Photogenerated Holes in Monolayer C ₂ N. Journal of Physical Chemistry Letters, 2022, 13, 3332-3337.	4.6	7
6	A review of bipolar magnetic semiconductors from theoretical aspects. Fundamental Research, 2022, 2, 511-521.	3.3	19
7	Bipolar Magnetic Molecules for Spinâ€₽olarized 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	Two-Dimensional Multifunctional Metal–Organic Framework with Intrinsic Bipolar Magnetic Semiconductivity and Negative Poisson's Ratio. ACS Applied Electronic Materials, 2022, 4, 3198-3204.	4.3	6
10	Efficient interlayer charge release for high-performance layered thermoelectrics. National Science Review, 2021, 8, nwaa085.	9.5	15
11	Strain-Stabilized Metastable Face-Centered Tetragonal Gold Overlayer for Efficient CO ₂ Electroreduction. Nano Letters, 2021, 21, 1003-1010.	9.1	32
12	CrSbS ₃ monolayer: a potential phase transition ferromagnetic semiconductor. Nanoscale, 2021, 13, 14067-14072.	5.6	5
13	A single-molecule electrical approach for amino acid detection and chirality recognition. Science Advances, 2021, 7, .	10.3	43
14	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
15	Thickness Dependent Magnetic Transition in Few Layer 1T Phase CrTe ₂ . Journal of Physical Chemistry Letters, 2021, 12, 6847-6851.	4.6	19
16	Unveiling the full reaction path of the Suzuki–Miyaura cross-coupling in a single-molecule junction. Nature Nanotechnology, 2021, 16, 1214-1223.	31.5	46
17	A rationally designed two-dimensional MoSe ₂ /Ti ₂ CO ₂ heterojunction for photocatalytic overall water splitting: simultaneously suppressing electron–hole recombination and photocorrosion. Chemical Science, 2021, 12, 2863-2869.	7.4	82
18	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

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19	Designing Two-Dimensional Versatile Room-Temperature Ferromagnets via Assembling Large-Scale Magnetic Quantum Dots. Nano Letters, 2021, 21, 9816-9823.	9.1	11
20	High Curie Temperature and Intrinsic Ferromagnetic Half-Metallicity in Mn ₂ X ₃ (X = S, Se, Te) Nanosheets. Journal of Physical Chemistry Letters, 2021, 12, 11790-11794.	4.6	14
21	Largeâ€Spinâ€Gap Nodalâ€Line Halfâ€Metal and Highâ€Temperature Ferromagnetic Semiconductor in Cr ₂ X ₃ (X=O,S,Se) Monolayers. Advanced Electronic Materials, 2020, 6, 1900490.	5.1	27
22	Excitons in bent black phosphorus nanoribbons: multiple excitonic funnels. Materials Today Advances, 2020, 7, 100096.	5.2	6
23	Proposed mechanical method for switching the spin transport channel in two-dimensional magnetic metal–magnetic semiconductor van der Waals contacts. Nanoscale Horizons, 2020, 5, 1496-1499.	8.0	5
24	Two-Dimensional Multifunctional Metal–Organic Frameworks with Simultaneous Ferro-/Ferrimagnetism and Vertical Ferroelectricity. Journal of Physical Chemistry Letters, 2020, 11, 4193-4197.	4.6	30
25	Prediction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnSiTe</mml:mi><mml:mn>3< as an intrinsic layered half-metal. Physical Review B, 2020, 101, .</mml:mn></mml:msub></mml:math 	/mm <mark>lana</mark> n><,	/mmt:msub><
26	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
27	Atomic-Level Construction of Tensile-Strained PdFe Alloy Surface toward Highly Efficient Oxygen Reduction Electrocatalysis. Nano Letters, 2020, 20, 1403-1409.	9.1	89
28	Are pyridinium ylides radicals?. Chemical Communications, 2020, 56, 11287-11290.	4.1	8
29	Room-Temperature Ferromagnetism in Transition Metal Embedded Borophene Nanosheets. Journal of Physical Chemistry Letters, 2019, 10, 4417-4421.	4.6	26
30	Significantly Enhanced Charge Separation in Rippled Monolayer Graphitic C 3 N 4. ChemCatChem, 2019, 11, 6252-6257.	3.7	9
31	Computational Design of Oneâ€Dimensional Ferromagnetic Semiconductors in Transition Metal Embedded Stannaspherene Nanowires. Chinese Journal of Chemistry, 2019, 37, 1021-1024.	4.9	7
32	Revealing Charge―and Temperatureâ€Dependent Movement Dynamics and Mechanism of Individual Molecular Machines. Small Methods, 2019, 3, 1900464.	8.6	21
33	The Contacts of the Monolayer Semiconductor C ₂ N with 2D Metal Electrodes. Advanced Theory and Simulations, 2019, 2, 1800161.	2.8	19
34	Unconventional p–d Hybridization Interaction in PtGa Ultrathin Nanowires Boosts Oxygen Reduction Electrocatalysis. Journal of the American Chemical Society, 2019, 141, 18083-18090.	13.7	216
35	Proposal of a stable B ₃ S nanosheet as an efficient hydrogen evolution catalyst. Journal of Materials Chemistry A, 2019, 7, 3752-3756.	10.3	41
36	Toward Room-Temperature Magnetic Semiconductors in Two-Dimensional Ferrimagnetic Organometallic Lattices. Journal of Physical Chemistry Letters, 2019, 10, 2439-2444.	4.6	39

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37	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, .	7.9	25
38	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
39	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
40	Direct observation of single-molecule hydrogen-bond dynamics with single-bond resolution. Nature Communications, 2018, 9, 807.	12.8	78
41	A high performance catalyst for methane conversion to methanol: graphene supported single atom Co. Chemical Communications, 2018, 54, 2284-2287.	4.1	57
42	The roles of buckled geometry and water environment in the excitonic properties of graphitic C ₃ N ₄ . Nanoscale, 2018, 10, 3738-3743.	5.6	17
43	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
44	Frontispiz: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. Angewandte Chemie, 2018, 130, .	2.0	0
45	Frontispiece: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. Angewandte Chemie - International Edition, 2018, 57, .	13.8	0
46	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
47	Tuning Charge Transport in Aromaticâ€Ring Singleâ€Molecule Junctions via Ionic‣iquid Gating. Angewandte Chemie, 2018, 130, 14222-14227.	2.0	22
48	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
49	Tuning Charge Transport in Aromaticâ€Ring Singleâ€Molecule Junctions via Ionic‣iquid Gating. Angewandte Chemie - International Edition, 2018, 57, 14026-14031.	13.8	52
50	Lowâ€dimensional halfâ€metallic materials: theoretical simulations and design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1314.	14.6	47
51	Γ̈́-Phosphorene: a new allotrope of phosphorene. Physical Chemistry Chemical Physics, 2017, 19, 2402-2408.	2.8	65
52	δ-Phosphorene: a two dimensional material with a highly negative Poisson's ratio. Nanoscale, 2017, 9, 850-855.	5.6	150
53	BP ₅ monolayer with multiferroicity and negative Poisson's ratio: a prediction by global optimization method. 2D Materials, 2017, 4, 045020.	4.4	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. Journal of Materials Chemistry A, 2017, 5, 24972-24980.	10.3	90

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55	The g ₃ N ₄ /C ₂ N Nanocomposite: A g ₃ N ₄ â€Based Waterâ€&plitting Photocatalyst with Enhanced Energy Efficiency. ChemPhysChem, 2016, 17, 2100-2104.	2.1	118
56	A many-body <i>GW</i> + BSE investigation of electronic and optical properties of C2N. Applied Physics Letters, 2016, 109, .	3.3	51
57	First-principles design of spintronics materials. National Science Review, 2016, 3, 365-381.	9.5	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.	10.3	108
59	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. Physical Review B, 2015, 92, .	3.2	23
60	Comparative Study on Electronic Structures of Sc and Ti Contacts with Monolayer and Multilayer MoS ₂ . ACS Applied Materials & Interfaces, 2015, 7, 12981-12987.	8.0	36
61	Electrical control of carriers' spin orientation in the FeVTiSi Heusler alloy. Journal of Materials Chemistry C, 2015, 3, 2563-2567.	5.5	30
62	Single layer of MX ₃ (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
63	SiN-SiC nanofilm: A nano-functional ceramic with bipolar magnetic semiconducting character. Applied Physics Letters, 2014, 104, .	3.3	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.	3.7	23
65	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. Physical Review Letters, 2014, 112, 018301.	7.8	237
66	CrXTe ₃ (X = Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors. Journal of Materials Chemistry C, 2014, 2, 7071.	5.5	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.	13.7	88
68	Half-Metallicity in MnPSe ₃ Exfoliated Nanosheet with Carrier Doping. Journal of the American Chemical Society, 2014, 136, 11065-11069.	13.7	353
69	Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. Physical Chemistry Chemical Physics, 2013, 15, 15793.	2.8	78
70	Control of spin in a La(Mn,Zn)AsO alloy by carrier doping. Journal of Materials Chemistry C, 2013, 1, 7197.	5.5	17
71	Semihydrogenated BN Sheet: A Promising Visible-light Driven Photocatalyst for Water Splitting. Scientific Reports, 2013, 3, 1858.	3.3	127
72	Bipolar magnetic semiconductors: a new class of spintronics materials. Nanoscale, 2012, 4, 5680.	5.6	241