Lei Shen

List of Publications by Year
in descending order

100 papers	5,709 citations	81743 39 h-index	76769 74 g-index
102 all docs	102 docs citations	102 times ranked	7427 citing authors

#	Article	IF	Citations
1	Generation and Enhancement of Valley Polarization in Monolayer Chromium Dichalcogenides. Journal of Superconductivity and Novel Magnetism, 2022, 35, 787.	0.8	1
2	Giant tunnelling electroresistance through 2D sliding ferroelectric materials. Materials Horizons, 2022, 9, 1422-1430.	6.4	23
3	Data-driven discovery of high performance layered van der Waals piezoelectric NbOI2. Nature Communications, 2022, 13, 1884.	5.8	22
4	Epitaxial Growth of Ultraflat Bismuthene with Large Topological Band Inversion Enabled by Substrate-Orbital-Filtering Effect. ACS Nano, 2022, 16, 1436-1443.	7.3	16
5	Formation of magnetic anionic electrons by hole doping. Journal of Materials Chemistry C, 2022, 10, 7674-7679.	2.7	3
6	Boost the large driving photovoltages for overall water splitting in direct Z-scheme heterojunctions by interfacial polarization. Catalysis Science and Technology, 2022, 12, 3614-3621.	2.1	10
7	High-Throughput Computational Discovery and Intelligent Design of Two-Dimensional Functional Materials for Various Applications. Accounts of Materials Research, 2022, 3, 572-583.	5.9	21
8	Protected valley states and generation of valley- and spin-polarized current in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>M</mml:mi> Physical Review B, 2022, 105, .	1.1	21
9	Developing Dipole-scheme heterojunction photocatalysts. Applied Surface Science, 2022, 599, 153942.	3.1	6
10	Singleâ€Crystalline TiO₂(B) Nanobelts with Unusual Large Exposed {100} Facets and Enhanced Liâ€Storage Capacity. Advanced Functional Materials, 2021, 31, 2002187.	7.8	25
11	Boosting the photon absorption, exciton dissociation, and photocatalytic hydrogen- and oxygen-evolution reactions by built-in electric fields in Janus platinum dichalcogenides. Journal of Materials Chemistry C, 2021, 9, 15026-15033.	2.7	28
12	Prominent nonequilibrium effects beyond the standard first-principles approach in nanoscale electronic devices. Nanoscale Horizons, 2021, 6, 801-808.	4.1	3
13	Effect of Acetylene Links on Electronic and Optical Properties of Semiconducting Graphynes. ACS Omega, 2021, 6, 10997-11004.	1.6	5
14	Recent progress and challenges in magnetic tunnel junctions with 2D materials for spintronic applications. Applied Physics Reviews, 2021, 8, .	5.5	74
15	Origin and enhancement of the spin Hall angle in the Weyl semimetals LaAlSi and LaAlGe. Physical Review B, 2021, 104, .	1.1	14
16	Quasiâ€Paired Pt Atomic Sites on Mo₂C Promoting Selective Fourâ€Electron Oxygen Reduction. Advanced Science, 2021, 8, e2101344.	5.6	29
17	A first principles study of uniaxial strain-stabilized longâ€“range ferromagnetic ordering in electrenes. Journal of Materials Chemistry C, 2021, 9, 16576-16580.	2.7	5
18	Tunable Rashba spin-orbit coupling and its interplay with multiorbital effect and magnetic ordering at oxide interfaces. Physical Review B, 2021, 104, .	1.1	8

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19	Self-Assembly of a Two-Dimensional Sheet with Ta@Si₁₆ Superatoms and Its Magnetic and Photocatalytic Properties. Journal of Physical Chemistry C, 2020, 124, 6861-6870.	1.5	18
20	High-throughput screening of transition metal single atom catalysts anchored on molybdenum disulfide for nitrogen fixation. Nano Energy, 2020, 68, 104304.	8.2	136
21	Tailoring magnetic order via atomically stacking 3d/5d electrons to achieve high-performance spintronic devices. Applied Physics Reviews, 2020, 7, .	5.5	18
22	Multimodal Plant Healthcare Flexible Sensor System. ACS Nano, 2020, 14, 10966-10975.	7.3	129
23	Negative Pressure Pyrolysis Induced Highly Accessible Single Sites Dispersed on 3D Graphene Frameworks for Enhanced Oxygen Reduction. Angewandte Chemie, 2020, 132, 20645-20649.	1.6	16
24	Negative Pressure Pyrolysis Induced Highly Accessible Single Sites Dispersed on 3D Graphene Frameworks for Enhanced Oxygen Reduction. Angewandte Chemie - International Edition, 2020, 59, 20465-20469.	7.2	104
25	Gas Sensors: Highly Sensitive and Selective Sensors for CF₄ Gas Molecules Based on Twoâ€Node Hollow Fullerene (Adv. Mater. Interfaces 20/2020). Advanced Materials Interfaces, 2020, 7, 2070114.	1.9	0
26	Highly Sensitive and Selective Sensors for CF 4 Gas Molecules Based on Twoâ€Node Hollow Fullerene. Advanced Materials Interfaces, 2020, 7, 2000985.	1.9	4
27	Atomic-orbital-free intrinsic ferromagnetism in electrenes. Physical Review B, 2020, 102, .	1.1	34
28	High-Throughput Identification of Exfoliable Two-Dimensional Materials with Active Basal Planes for Hydrogen Evolution. ACS Energy Letters, 2020, 5, 2313-2321.	8.8	54
29	Intrinsic skyrmions in monolayer Janus magnets. Physical Review B, 2020, 101, .	1.1	94
30	Synergizing Mo Single Atoms and Mo₂C Nanoparticles on CNTs Synchronizes Selectivity and Activity of Electrocatalytic N₂ Reduction to Ammonia. Advanced Materials, 2020, 32, e2002177.	11.1	190
31	Diverse Transport Behaviors in Cyclo[18]carbon-Based Molecular Devices. Journal of Physical Chemistry Letters, 2020, 11, 2611-2617.	2.1	52
32	Interfacial-hybridization-modified Ir ferromagnetism and electronic structure in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>LaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> superlattices. Physical Review Research, 2020, 2, .	1.3	10
33	Taper-shaped carbon based spin filter. Applied Surface Science, 2019, 495, 143501.	3.1	8
34	Electrically controlled spin-switch and evolution of Hanle spin precession in graphene. 2D Materials, 2019, 6, 035042.	2.0	12
35	Copper Single Atoms Anchored in Porous Nitrogen-Doped Carbon as Efficient pH-Universal Catalysts for the Nitrogen Reduction Reaction. ACS Catalysis, 2019, 9, 10166-10173.	5.5	284
36	Stimulated Electrocatalytic Hydrogen Evolution Activity of MOFâ€Derived MoS₂ Basal Domains via Charge Injection through Surface Functionalization and Heteroatom Doping. Advanced Science, 2019, 6, 1900140.	5.6	73

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37	Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. Journal of Materials Chemistry C, 2019, 7, 8868-8873.	2.7	52
38	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. Scientific Data, 2019, 6, 86.	2.4	201
39	Titelbild: Disorder Engineering in Monolayer Nanosheets Enabling Photothermic Catalysis for Full Solar Spectrum (250â€“2500â€…nm) Harvesting (Angew. Chem. 10/2019). Angewandte Chemie, 2019, 131, 2933-2933.	1.6	0
40	Discovery of Hidden Classes of Layered Electrides by Extensive High-Throughput Material Screening. Chemistry of Materials, 2019, 31, 1860-1868.	3.2	39
41	Suppression of Defect-Induced Quenching via Chemical Potential Tuning: A Theoretical Solution for Enhancing Lanthanide Luminescence. Journal of Physical Chemistry C, 2019, 123, 11151-11161.	1.5	26
42	Disorder Engineering in Monolayer Nanosheets Enabling Photothermic Catalysis for Full Solar Spectrum (250â€“2500â€…nm) Harvesting. Angewandte Chemie, 2019, 131, 3109-3113.	1.6	9
43	Unravelling uniaxial strain effects on electronic correlations, hybridization and bonding in transition metal oxides. Acta Materialia, 2019, 164, 618-626.	3.8	3
44	Disorder Engineering in Monolayer Nanosheets Enabling Photothermic Catalysis for Full Solar Spectrum (250â€“2500â€…nm) Harvesting. Angewandte Chemie - International Edition, 2019, 58, 3077-3081.	7.2	100
45	Efficient charge-spin conversion and magnetization switching through the Rashba effect at topological-insulator/Ag interfaces. Physical Review B, 2018, 97, .	1.1	53
46	Large valley splitting in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">WS</mml:mi><mml:mn mathvariant="bold">2</mml:mn></mml:msub></mml:math> by proximity coupling to an insulating antiferromagnetic substrate. Physical Review B, 2018, 97, .	1.1	134
47	Ti1-Sn O2 nanofilms: Layer-by-layer deposition with extended Sn solubility and characterization. Applied Surface Science, 2018, 428, 710-717.	3.1	7
48	Identification of Facetâ€Governing Reactivity in Hematite for Oxygen Evolution. Advanced Materials, 2018, 30, e1804341.	11.1	96
49	High-Throughput Computational Screening of Vertical 2D van der Waals Heterostructures for High-efficiency Excitonic Solar Cells. ACS Applied Materials & Interfaces, 2018, 10, 32142-32150.	4.0	75
50	Ferromagnetism and matrix-dependent charge transfer in strained LaMnO₃â€“LaCoO₃ superlattices. Materials Research Letters, 2018, 6, 501-507.	4.1	13
51	One-dimensional thermoelectrics induced by Rashba spin-orbit coupling in two-dimensional BiSb monolayer. Nano Energy, 2018, 52, 163-170.	8.2	41
52	Robust two-dimensional bipolar magnetic semiconductors by defect engineering. Journal of Materials Chemistry C, 2018, 6, 8435-8443.	2.7	26
53	Prospects of spintronics based on <scp>2D</scp> materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1313.	6.2	161
54	Unveiling the role of Co-O-Mg bond in magnetic anisotropy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pt</mml:mi><mml:mo>/</mml:mo><mml:mi>Co</mml:mi><mml:m using atomically controlled deposition and in situ electrical measurement. Physical Review B, 2017, 95, .	1.1	11

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55	Pressure induced topological phase transition in layered Bi₂S₃. Physical Chemistry Chemical Physics, 2017, 19, 29372-29380.	1.3	18
56	Si₂₄: An Efficient Solar Cell Material. Journal of Physical Chemistry C, 2017, 121, 15574-15579.	1.5	17
57	Interface-Induced Enhancement of Ferromagnetism in Insulating LaMnO₃ Ultrathin Films. ACS Applied Materials & Interfaces, 2017, 9, 44931-44937.	4.0	23
58	Achieving giant tunneling electroresistance and magnetoresistance by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></m barrier and Heusler alloy electrode. Physical Review Materials, 2017, 1, .	0.9	8
59	2D Materials and Devices for Spintronics: First-Principles Studies. , 2016, , .		0
60	Surface defect passivation of MoS2 by sulfur, selenium, and tellurium. Journal of Applied Physics, 2016, 119, .	1.1	15
61	Heterostructures of phosphorene and transition metal dichalcogenides for excitonic solar cells: A first-principles study. Applied Physics Letters, 2016, 108, .	1.5	90
62	Chemisorption-induced n-doping of MoS2 by oxygen. Applied Physics Letters, 2016, 108, .	1.5	71
63	Tuning polarization states and interface properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn><m by metal capping layers. Physical Review B, 2016, 93, .	1.1	5
64	Giant tunneling electroresistance induced by ferroelectrically switchable two-dimensional electron gas at nonpolar<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></m Physical Review B, 2016, 94, .	1.1	15
65	Tailoring Selfâ€Polarization of BaTiO₃ Thin Films by Interface Engineering and Flexoelectric Effect. Advanced Materials Interfaces, 2016, 3, 1600737.	1.9	37
66	Ferromagnetism of wide-bandgap semiconductor surfaces: Mg-doped AlN. Japanese Journal of Applied Physics, 2015, 54, 110302.	0.8	2
67	Electrically Tunable In-Plane Anisotropic Magnetoresistance in Topological Insulator BiSbTeSe₂ Nanodevices. Nano Letters, 2015, 15, 2061-2066.	4.5	56
68	Magnetism in phosphorene: Interplay between vacancy and strain. Applied Physics Letters, 2015, 107, .	1.5	46
69	Electronic and transport properties of phosphorene nanoribbons. Physical Review B, 2015, 92, .	1.1	145
70	Topological Properties Determined by Atomic Buckling in Self-Assembled Ultrathin Bi(110). Nano Letters, 2015, 15, 80-87.	4.5	191
71	Magnetocrystalline anisotropy and its electric-field-assisted switching of Heusler-compound-based perpendicular magnetic tunnel junctions. New Journal of Physics, 2014, 16, 103033.	1.2	43
72	Efficient Spin Injection into Graphene through a Tunnel Barrier: Overcoming the Spin-Conductance Mismatch. Physical Review Applied, 2014, 2, .	1.5	39

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73	Experimental evidences of topological surface states of Î²-Ag2Te. AIP Advances, 2013, 3, 032123.	0.6	36
74	On the origin of giant magnetocaloric effect and thermal hysteresis in multifunctional Î±-FeRh thin films. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 3052-3059.	0.9	33
75	Roomâ€Temperature Ferromagnetism in ZnOâ€Encapsulated 1.9 nm FePt₃ Nanoparticleâ€“Composite Thin Films with Giant Interfacial Anisotropy. Advanced Materials, 2013, 25, 1639-1645.	11.1	9
76	High-performance giant-magnetoresistance junctions based on the all-Heusler architecture with matched energy bands and Fermi surfaces. Applied Physics Letters, 2013, 102, 152403.	1.5	15
77	Boron diffusion induced symmetry reduction and scattering in CoFeB/MgO/CoFeB magnetic tunnel junctions. Physical Review B, 2013, 87, .	1.1	33
78	Simultaneous Magnetic and Charge Doping of Topological Insulators with Carbon. Physical Review Letters, 2013, 111, 236803.	2.9	12
79	Magnetic and transport properties of Mn3â^'xGa/MgO/Mn3â^'xGa magnetic tunnel junctions: A first-principles study. Applied Physics Letters, 2012, 100, .	1.5	49
80	Soft layer driven switching of microwave-assisted magnetic recording on segmented perpendicular media. Journal of Applied Physics, 2012, 111, .	1.1	6
81	Origin of Long-Range Ferromagnetic Ordering in Metalâ€“Organic Frameworks with Antiferromagnetic Dimeric-Cu(II) Building Units. Journal of the American Chemical Society, 2012, 134, 17286-17290.	6.6	86
82	Systematic study of ferroelectric, interfacial, oxidative, and doping effects on conductance of Pt/BaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/Pt ferroelectic tunnel junctions. Physical Review B, 2012, 85, .	1.1	23
83	DATA STORAGE: REVIEW OF HEUSLER COMPOUNDS. Spin, 2012, 02, 1230006.	0.6	73
84	Electron transmission modes in electrically biased graphene nanoribbons and their effects on device performance. Physical Review B, 2012, 86, .	1.1	48
85	Charge and spin transport in graphene-based heterostructure. Applied Physics Letters, 2011, 98, 053101.	1.5	62
86	Graphene-based bipolar spin diode and spin transistor: Rectification and amplification of spin-polarized current. Physical Review B, 2011, 83, .	1.1	145
87	Graphene-based spin logic gates. Applied Physics Letters, 2011, 98, .	1.5	59
88	The Effect of Introduced Defects on Saturation Magnetization and Magnetic Anisotropy Field of L1$ _{0}$ FePt. IEEE Transactions on Magnetics, 2011, 47, 2422-2424.	1.2	4
89	FePt Grain Size Limit and Required Switching Field in the Presence of Surface Anisotropy. IEEE Transactions on Magnetics, 2011, 47, 3809-3812.	1.2	1
90	Origin of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi>d</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:mrow></mml:math>magn in II-VI and III-V semiconductors by substitutional doping at anion site. Physical Review B, 2010, 81, .	1.1	119

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91	Electron Transport Properties of Atomic Carbon Nanowires between Graphene Electrodes. Journal of the American Chemical Society, 2010, 132, 11481-11486.	6.6	181
92	Oxidization states of metal atoms in linear bimetallic multi-sandwich molecules Vn(FeCp2)(n+1) and magnetic moment enhancement mechanism of its 1D wire. Physical Chemistry Chemical Physics, 2010, 12, 4555.	1.3	22
93	Chemically Linked AuNPâ^'Alkane Network for Enhanced Photoemission and Field Emission. ACS Nano, 2009, 3, 2722-2730.	7.3	21
94	Effects of edge passivation by hydrogen on electronic structure of armchair graphene nanoribbon and band gap engineering. Applied Physics Letters, 2009, 94, .	1.5	112
95	Geometry Dependent Iâ^'V Characteristics of Silicon Nanowires. Nano Letters, 2008, 8, 3662-3667.	4.5	35
96	One-Dimensional Ironâ^'Cyclopentadienyl Sandwich Molecular Wire with Half Metallic, Negative Differential Resistance and High-Spin Filter Efficiency Properties. Journal of the American Chemical Society, 2008, 130, 4023-4027.	6.6	185
97	Charge-Transfer-Based Mechanism for Half-Metallicity and Ferromagnetism in One-Dimensional Organometallic Sandwich Molecular Wires. Journal of the American Chemical Society, 2008, 130, 13956-13960.	6.6	118
98	Interface properties of Ge3N4/Ge(111): Ab initio and x-ray photoemission spectroscopy study. Applied Physics Letters, 2008, 93, 222907.	1.5	16
99	Possible efficient p-type doping of AlN using Be: An ab initio study. Applied Physics Letters, 2007, 91, 152110.	1.5	18
100	Room-Temperature Ferromagnetism in Carbon-Doped ZnO. Physical Review Letters, 2007, 99, 127201.	2.9	775