

# Lei Shen

## List of Publications by Year in descending order

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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	Room-Temperature Ferromagnetism in Carbon-Doped ZnO. <i>Physical Review Letters</i> , 2007, 99, 127201.	2.9	775
2	Copper Single Atoms Anchored in Porous Nitrogen-Doped Carbon as Efficient pH-Universal Catalysts for the Nitrogen Reduction Reaction. <i>ACS Catalysis</i> , 2019, 9, 10166-10173.	5.5	284
3	2DMatPedia, an open computational database of two-dimensional materials from top-down and bottom-up approaches. <i>Scientific Data</i> , 2019, 6, 86.	2.4	201
4	Topological Properties Determined by Atomic Buckling in Self-Assembled Ultrathin Bi(110). <i>Nano Letters</i> , 2015, 15, 80-87.	4.5	191
5	Synergizing Mo Single Atoms and Mo <sub>2</sub> C Nanoparticles on CNTs Synchronizes Selectivity and Activity of Electrocatalytic N <sub>2</sub> Reduction to Ammonia. <i>Advanced Materials</i> , 2020, 32, e2002177.	11.1	190
6	One-Dimensional Iron <sup>II</sup> -Cyclopentadienyl Sandwich Molecular Wire with Half Metallic, Negative Differential Resistance and High-Spin Filter Efficiency Properties. <i>Journal of the American Chemical Society</i> , 2008, 130, 4023-4027.	6.6	185
7	Electron Transport Properties of Atomic Carbon Nanowires between Graphene Electrodes. <i>Journal of the American Chemical Society</i> , 2010, 132, 11481-11486.	6.6	181
8	Prospects of spintronics based on 2D materials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2017, 7, e1313.	6.2	161
9	Graphene-based bipolar spin diode and spin transistor: Rectification and amplification of spin-polarized current. <i>Physical Review B</i> , 2011, 83, .	1.1	145
10	Electronic and transport properties of phosphorene nanoribbons. <i>Physical Review B</i> , 2015, 92, .	1.1	145
11	High-throughput screening of transition metal single atom catalysts anchored on molybdenum disulfide for nitrogen fixation. <i>Nano Energy</i> , 2020, 68, 104304.	8.2	136
12	Large valley splitting in monolayer WS <sub>2</sub> by proximity coupling to an insulating antiferromagnetic substrate. <i>Physical Review B</i> , 2018, 97, .	1.1	134
13	Multimodal Plant Healthcare Flexible Sensor System. <i>ACS Nano</i> , 2020, 14, 10966-10975.	7.3	129
14	Origin of d <sup>0</sup> magnon in II-VI and III-V semiconductors by substitutional doping at anion site. <i>Physical Review B</i> , 2010, 81, .	1.1	129
15	Charge-Transfer-Based Mechanism for Half-Metallicity and Ferromagnetism in One-Dimensional Organometallic Sandwich Molecular Wires. <i>Journal of the American Chemical Society</i> , 2008, 130, 13956-13960.	6.6	118
16	Effects of edge passivation by hydrogen on electronic structure of armchair graphene nanoribbon and band gap engineering. <i>Applied Physics Letters</i> , 2009, 94, .	1.5	112
17	Negative Pressure Pyrolysis Induced Highly Accessible Single Sites Dispersed on 3D Graphene Frameworks for Enhanced Oxygen Reduction. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20465-20469.	7.2	104
18	Disorder Engineering in Monolayer Nanosheets Enabling Photothermic Catalysis for Full Solar Spectrum (250–2500 nm) Harvesting. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3077-3081.	7.2	100

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19	Identification of Facet-Governing Reactivity in Hematite for Oxygen Evolution. <i>Advanced Materials</i> , 2018, 30, e1804341.	11.1	96
20	Intrinsic skyrmions in monolayer Janus magnets. <i>Physical Review B</i> , 2020, 101, .	1.1	94
21	Heterostructures of phosphorene and transition metal dichalcogenides for excitonic solar cells: A first-principles study. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	90
22	Origin of Long-Range Ferromagnetic Ordering in Metal-Organic Frameworks with Antiferromagnetic Dimeric-Cu(II) Building Units. <i>Journal of the American Chemical Society</i> , 2012, 134, 17286-17290.	6.6	86
23	High-Throughput Computational Screening of Vertical 2D van der Waals Heterostructures for High-efficiency Excitonic Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 32142-32150.	4.0	75
24	Recent progress and challenges in magnetic tunnel junctions with 2D materials for spintronic applications. <i>Applied Physics Reviews</i> , 2021, 8, .	5.5	74
25	DATA STORAGE: REVIEW OF HEUSLER COMPOUNDS. <i>Spin</i> , 2012, 02, 1230006.	0.6	73
26	Stimulated Electrocatalytic Hydrogen Evolution Activity of MOF-Derived MoS <sub>2</sub> Basal Domains via Charge Injection through Surface Functionalization and Heteroatom Doping. <i>Advanced Science</i> , 2019, 6, 1900140.	5.6	73
27	Chemisorption-induced <i>n</i> -doping of MoS <sub>2</sub> by oxygen. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	71
28	Charge and spin transport in graphene-based heterostructure. <i>Applied Physics Letters</i> , 2011, 98, 053101.	1.5	62
29	Graphene-based spin logic gates. <i>Applied Physics Letters</i> , 2011, 98, .	1.5	59
30	Electrically Tunable In-Plane Anisotropic Magnetoresistance in Topological Insulator BiSbTeSe <sub>2</sub> Nanodevices. <i>Nano Letters</i> , 2015, 15, 2061-2066.	4.5	56
31	High-Throughput Identification of Exfoliable Two-Dimensional Materials with Active Basal Planes for Hydrogen Evolution. <i>ACS Energy Letters</i> , 2020, 5, 2313-2321.	8.8	54
32	Efficient charge-spin conversion and magnetization switching through the Rashba effect at topological-insulator/Ag interfaces. <i>Physical Review B</i> , 2018, 97, .	1.1	53
33	Tungsten boride: a 2D multiple Dirac semimetal for the hydrogen evolution reaction. <i>Journal of Materials Chemistry C</i> , 2019, 7, 8868-8873.	2.7	52
34	Diverse Transport Behaviors in Cyclo[18]carbon-Based Molecular Devices. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2611-2617.	2.1	52
35	Magnetic and transport properties of Mn <sub>3</sub> xGa/MgO/Mn <sub>3</sub> xGa magnetic tunnel junctions: A first-principles study. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	49
36	Electron transmission modes in electrically biased graphene nanoribbons and their effects on device performance. <i>Physical Review B</i> , 2012, 86, .	1.1	48

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37	Magnetism in phosphorene: Interplay between vacancy and strain. <i>Applied Physics Letters</i> , 2015, 107, .	1.5	46
38	Magnetocrystalline anisotropy and its electric-field-assisted switching of Heusler-compound-based perpendicular magnetic tunnel junctions. <i>New Journal of Physics</i> , 2014, 16, 103033.	1.2	43
39	One-dimensional thermoelectrics induced by Rashba spin-orbit coupling in two-dimensional BiSb monolayer. <i>Nano Energy</i> , 2018, 52, 163-170.	8.2	41
40	Efficient Spin Injection into Graphene through a Tunnel Barrier: Overcoming the Spin-Conductance Mismatch. <i>Physical Review Applied</i> , 2014, 2, .	1.5	39
41	Discovery of Hidden Classes of Layered Electrides by Extensive High-Throughput Material Screening. <i>Chemistry of Materials</i> , 2019, 31, 1860-1868.	3.2	39
42	Tailoring Self-Polarization of BaTiO <sub>3</sub> Thin Films by Interface Engineering and Flexoelectric Effect. <i>Advanced Materials Interfaces</i> , 2016, 3, 1600737.	1.9	37
43	Experimental evidences of topological surface states of $\hat{I}^2$ -Ag <sub>2</sub> Te. <i>AIP Advances</i> , 2013, 3, 032123.	0.6	36
44	Geometry Dependent I <sup>~</sup> V Characteristics of Silicon Nanowires. <i>Nano Letters</i> , 2008, 8, 3662-3667.	4.5	35
45	Atomic-orbital-free intrinsic ferromagnetism in electrenes. <i>Physical Review B</i> , 2020, 102, .	1.1	34
46	On the origin of giant magnetocaloric effect and thermal hysteresis in multifunctional $\hat{I}^{\pm}$ -FeRh thin films. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2013, 377, 3052-3059.	0.9	33
47	Boron diffusion induced symmetry reduction and scattering in CoFeB/MgO/CoFeB magnetic tunnel junctions. <i>Physical Review B</i> , 2013, 87, .	1.1	33
48	Quasi-Paired Pt Atomic Sites on Mo <sub>2</sub> C Promoting Selective Four-Electron Oxygen Reduction. <i>Advanced Science</i> , 2021, 8, e2101344.	5.6	29
49	Boosting the photon absorption, exciton dissociation, and photocatalytic hydrogen- and oxygen-evolution reactions by built-in electric fields in Janus platinum dichalcogenides. <i>Journal of Materials Chemistry C</i> , 2021, 9, 15026-15033.	2.7	28
50	Robust two-dimensional bipolar magnetic semiconductors by defect engineering. <i>Journal of Materials Chemistry C</i> , 2018, 6, 8435-8443.	2.7	26
51	Suppression of Defect-Induced Quenching via Chemical Potential Tuning: A Theoretical Solution for Enhancing Lanthanide Luminescence. <i>Journal of Physical Chemistry C</i> , 2019, 123, 11151-11161.	1.5	26
52	Single-Crystalline TiO <sub>2</sub> (B) Nanobelts with Unusual Large Exposed {100} Facets and Enhanced Li <sup>+</sup> Storage Capacity. <i>Advanced Functional Materials</i> , 2021, 31, 2002187.	7.8	25
53	Systematic study of ferroelectric, interfacial, oxidative, and doping effects on conductance of Pt/BaTiO <sub>3</sub> /Pt ferroelectric tunnel junctions. <i>Physical Review B</i> , 2012, 85, .	1.1	23
54	Interface-Induced Enhancement of Ferromagnetism in Insulating LaMnO <sub>3</sub> Ultrathin Films. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 44931-44937.	4.0	23

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55	Giant tunnelling electroresistance through 2D sliding ferroelectric materials. <i>Materials Horizons</i> , 2022, 9, 1422-1430.	6.4	23
56	Oxidization states of metal atoms in linear bimetallic multi-sandwich molecules $V_n(\text{FeCp}_2)_{(n+1)}$ and magnetic moment enhancement mechanism of its 1D wire. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4555.	1.3	22
57	Data-driven discovery of high performance layered van der Waals piezoelectric NbOI <sub>2</sub> . <i>Nature Communications</i> , 2022, 13, 1884.	5.8	22
58	Chemically Linked AuNP@Alkane Network for Enhanced Photoemission and Field Emission. <i>ACS Nano</i> , 2009, 3, 2722-2730.	7.3	21
59	High-Throughput Computational Discovery and Intelligent Design of Two-Dimensional Functional Materials for Various Applications. <i>Accounts of Materials Research</i> , 2022, 3, 572-583.	5.9	21
60	Protected valley states and generation of valley- and spin-polarized current in monolayer $\text{M}_2\text{A}$ . <i>Physical Review B</i> , 2022, 105, .		
61	Possible efficient p-type doping of AlN using Be: An ab initio study. <i>Applied Physics Letters</i> , 2007, 91, 152110.	1.5	18
62	Pressure induced topological phase transition in layered $\text{Bi}_2\text{S}_3$ . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29372-29380.	1.3	18
63	Self-Assembly of a Two-Dimensional Sheet with Ta@Si <sub>16</sub> Superatoms and Its Magnetic and Photocatalytic Properties. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6861-6870.	1.5	18
64	Tailoring magnetic order via atomically stacking 3d <sup>5</sup> electrons to achieve high-performance spintronic devices. <i>Applied Physics Reviews</i> , 2020, 7, .	5.5	18
65	Si <sub>24</sub> : An Efficient Solar Cell Material. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15574-15579.	1.5	17
66	Interface properties of Ge <sub>3</sub> N <sub>4</sub> /Ge(111): <i>Ab initio</i> and x-ray photoemission spectroscopy study. <i>Applied Physics Letters</i> , 2008, 93, 222907.	1.5	16
67	Negative Pressure Pyrolysis Induced Highly Accessible Single Sites Dispersed on 3D Graphene Frameworks for Enhanced Oxygen Reduction. <i>Angewandte Chemie</i> , 2020, 132, 20645-20649.	1.6	16
68	Epitaxial Growth of Ultraflat Bismuthene with Large Topological Band Inversion Enabled by Substrate-Orbital-Filtering Effect. <i>ACS Nano</i> , 2022, 16, 1436-1443.	7.3	16
69	High-performance giant-magnetoresistance junctions based on the all-Heusler architecture with matched energy bands and Fermi surfaces. <i>Applied Physics Letters</i> , 2013, 102, 152403.	1.5	15
70	Surface defect passivation of MoS <sub>2</sub> by sulfur, selenium, and tellurium. <i>Journal of Applied Physics</i> , 2016, 119, .	1.1	15
71	Giant tunneling electroresistance induced by ferroelectrically switchable two-dimensional electron gas at nonpolar $\text{BaTiO}_3$ . <i>Physical Review B</i> , 2016, 94, .	1.1	15
72	Origin and enhancement of the spin Hall angle in the Weyl semimetals LaAlSi and LaAlGe. <i>Physical Review B</i> , 2021, 104, .	1.1	14

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73	Ferromagnetism and matrix-dependent charge transfer in strained $\text{LaMnO}_3/\text{LaCoO}_3$ superlattices. <i>Materials Research Letters</i> , 2018, 6, 501-507.	4.1	13
74	Simultaneous Magnetic and Charge Doping of Topological Insulators with Carbon. <i>Physical Review Letters</i> , 2013, 111, 236803.	2.9	12
75	Electrically controlled spin-switch and evolution of Hanle spin precession in graphene. <i>2D Materials</i> , 2019, 6, 035042.	2.0	12
76	Unveiling the role of Co-O-Mg bond in magnetic anisotropy of $\text{Pt}/\text{Co}$ using atomically controlled deposition and <i>in situ</i> electrical measurement. <i>Physical Review B</i> , 2017, 95, .	1.1	11
77	Interfacial-hybridization-modified Ir ferromagnetism and electronic structure in $\text{LaMnO}_3/\text{Ir}$ superlattices. <i>Physical Review Research</i> , 2020, 2, .	1.1	11
78	Boost the large driving photovoltages for overall water splitting in direct Z-scheme heterojunctions by interfacial polarization. <i>Catalysis Science and Technology</i> , 2022, 12, 3614-3621.	2.1	10
79	Room-temperature Ferromagnetism in ZnO-Encapsulated 1.9 nm $\text{FePt}_3$ Nanoparticle-Composite Thin Films with Giant Interfacial Anisotropy. <i>Advanced Materials</i> , 2013, 25, 1639-1645.	11.1	9
80	Disorder Engineering in Monolayer Nanosheets Enabling Photothermic Catalysis for Full Solar Spectrum (250-2500 nm) Harvesting. <i>Angewandte Chemie</i> , 2019, 131, 3109-3113.	1.6	9
81	Taper-shaped carbon based spin filter. <i>Applied Surface Science</i> , 2019, 495, 143501.	3.1	8
82	Tunable Rashba spin-orbit coupling and its interplay with multiorbital effect and magnetic ordering at oxide interfaces. <i>Physical Review B</i> , 2021, 104, .	1.1	8
83	Ti1-Sn O2 nanofilms: Layer-by-layer deposition with extended Sn solubility and characterization. <i>Applied Surface Science</i> , 2018, 428, 710-717.	3.1	7
84	Soft layer driven switching of microwave-assisted magnetic recording on segmented perpendicular media. <i>Journal of Applied Physics</i> , 2012, 111, .	1.1	6
85	Developing Dipole-scheme heterojunction photocatalysts. <i>Applied Surface Science</i> , 2022, 599, 153942.	3.1	6
86	Tuning polarization states and interface properties of $\text{BaTiO}_3/\text{Pt}$ by metal capping layers. <i>Physical Review B</i> , 2016, 93, .	1.1	6
87	Effect of Acetylene Links on Electronic and Optical Properties of Semiconducting Graphynes. <i>ACS Omega</i> , 2021, 6, 10997-11004.	1.6	5
88	A first principles study of uniaxial strain-stabilized long-range ferromagnetic ordering in electrenes. <i>Journal of Materials Chemistry C</i> , 2021, 9, 16576-16580.	2.7	5
89	The Effect of Introduced Defects on Saturation Magnetization and Magnetic Anisotropy Field of $\text{L1}_0$ $\text{FePt}$ . <i>IEEE Transactions on Magnetics</i> , 2011, 47, 2422-2424.	1.2	4
90	Highly Sensitive and Selective Sensors for CF <sub>4</sub> Gas Molecules Based on Two-Node Hollow Fullerene. <i>Advanced Materials Interfaces</i> , 2020, 7, 2000985.	1.9	4

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91	Unravelling uniaxial strain effects on electronic correlations, hybridization and bonding in transition metal oxides. <i>Acta Materialia</i> , 2019, 164, 618-626.	3.8	3
92	Prominent nonequilibrium effects beyond the standard first-principles approach in nanoscale electronic devices. <i>Nanoscale Horizons</i> , 2021, 6, 801-808.	4.1	3
93	Achieving giant tunneling electroresistance and magnetoresistance by $\text{BaTiO}_3$ barrier and Heusler alloy electrode. <i>Physical Review Materials</i> , 2017, 1, .	0.9	3
94	Formation of magnetic anionic electrons by hole doping. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7674-7679.	2.7	3
95	Ferromagnetism of wide-bandgap semiconductor surfaces: Mg-doped AlN. <i>Japanese Journal of Applied Physics</i> , 2015, 54, 110302.	0.8	2
96	FePt Grain Size Limit and Required Switching Field in the Presence of Surface Anisotropy. <i>IEEE Transactions on Magnetics</i> , 2011, 47, 3809-3812.	1.2	1
97	Generation and Enhancement of Valley Polarization in Monolayer Chromium Dichalcogenides. <i>Journal of Superconductivity and Novel Magnetism</i> , 2022, 35, 787.	0.8	1
98	2D Materials and Devices for Spintronics: First-Principles Studies. , 2016, , .		0
99	Titelbild: Disorder Engineering in Monolayer Nanosheets Enabling Photothermic Catalysis for Full Solar Spectrum (250-2500 nm) Harvesting ( <i>Angew. Chem.</i> 10/2019). <i>Angewandte Chemie</i> , 2019, 131, 2933-2933.	1.6	0
100	Gas Sensors: Highly Sensitive and Selective Sensors for $\text{CF}_4$ Gas Molecules Based on Two-Node Hollow Fullerene ( <i>Adv. Mater. Interfaces</i> 20/2020). <i>Advanced Materials Interfaces</i> , 2020, 7, 2070114.	1.9	0