

Qimin Yan

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

66

papers

3,781

citations

31

h-index

61

g-index

69

ext. papers

4,313

ext. citations

6.2

avg, IF

5.4

L-index

#	Paper	IF	Citations
66	Antisite defect qubits in monolayer transition metal dichalcogenides.. <i>Nature Communications</i> , 2022 , 13, 492	17.4	3
65	Copper Nanoplates for Printing Flexible High-Temperature Conductors. <i>ACS Applied Nano Materials</i> , 2022 , 5, 4028-4037	5.6	3
64	Structure motif-centric learning framework for inorganic crystalline systems. <i>Science Advances</i> , 2021 , 7,	14.3	2
63	Two-dimensional MX Dirac materials and quantum spin Hall insulators with tunable electronic and topological properties. <i>Nano Research</i> , 2021 , 14, 584-589	10	5
62	Monolayer 2D semiconducting tellurides for high-mobility electronics. <i>Physical Review Materials</i> , 2021 , 5,	3.2	3
61	Graph-based deep learning frameworks for molecules and solid-state materials. <i>Computational Materials Science</i> , 2021 , 195, 110332	3.2	1
60	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. <i>Chemistry of Materials</i> , 2021 , 33, 7242-7253	9.6	1
59	Hierarchically 3D Porous Ag Nanostructures Derived from Silver Benzenethiolate Nanoboxes: Enabling CO Reduction with a Near-Unity Selectivity and Mass-Specific Current Density over 500 A/g. <i>Nano Letters</i> , 2020 , 20, 2806-2811	11.5	29
58	Quantum anomalous Hall effect in two-dimensional magnetic insulator heterojunctions. <i>Npj Computational Materials</i> , 2020 , 6,	10.9	11
57	Auxetic two-dimensional transition metal selenides and halides. <i>Npj Computational Materials</i> , 2020 , 6,	10.9	6
56	Computational Study of a Novel 2D Ferromagnetic Metal: the Ce2C Monolayer. <i>Physica Status Solidi - Rapid Research Letters</i> , 2020 , 14, 2000324	2.5	1
55	High current carrying and thermal conductive copper-carbon conductors. <i>Nanotechnology</i> , 2019 , 30, 185301	3.1	5
54	Varying topological properties of two-dimensional honeycomb lattices composed of endohedral fullerenes. <i>Physical Review B</i> , 2019 , 100,	3.3	1
53	First-principles study of mechanical and electronic properties of bent monolayer transition metal dichalcogenides. <i>Physical Review Materials</i> , 2019 , 3,	3.2	14
52	Key role of antibonding electron transfer in bonding on solid surfaces. <i>Physical Review Materials</i> , 2019 , 3,	3.2	12
51	Chemisorption Can Reverse Defect-Defect Interaction on Heterogeneous Catalyst Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 7311-7317	6.4	7
50	Elastic Properties and Fracture Behaviors of Biaxially Deformed, Polymorphic MoTe. <i>Nano Letters</i> , 2019 , 19, 761-769	11.5	31

49	Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes. <i>Chemical Communications</i> , 2018 , 54, 4625-4628	5.8	0
48	Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 847-854	3.4	61
47	Data-driven material discovery for photocatalysis: a short review. <i>Journal of Semiconductors</i> , 2018 , 39, 071001	2.3	12
46	Identification of a functional point defect in SrTiO ₃ . <i>Physical Review Materials</i> , 2018 , 2,	3.2	13
45	Co-Mo-P Based Electrocatalyst for Superior Reactivity in the Alkaline Hydrogen Evolution Reaction. <i>ChemCatChem</i> , 2018 , 10, 4832-4837	5.2	19
44	Learning atoms for materials discovery. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E6411-E6417	11.5	103
43	Solar fuels photoanode materials discovery by integrating high-throughput theory and experiment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 3040-3043	11.5	111
42	Negative Poisson's ratio in 1T-type crystalline two-dimensional transition metal dichalcogenides. <i>Nature Communications</i> , 2017 , 8, 15224	17.4	84
41	Doping of thermoelectric PbSe with chemically inert secondary phase nanoparticles. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 10881-10887	7.1	21
40	Impact of carrier localization on recombination in InGaN quantum wells and the efficiency of nitride light-emitting diodes: Insights from theory and numerical simulations. <i>Applied Physics Letters</i> , 2017 , 111, 113501	3.4	44
39	Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments. <i>ACS Energy Letters</i> , 2017 , 2, 2307-2312	20.1	25
38	Rational design of molecular crystals for enhanced charge transfer properties. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 12338-12342	7.1	6
37	Prediction of Ideal Topological Semimetals with Triply Degenerate Points in the NaCu ₃ Te ₂ Family. <i>Physical Review Letters</i> , 2017 , 119, 256402	7.4	29
36	Prediction of TiRhAs as a Dirac nodal line semimetal via first-principles calculations. <i>Physical Review B</i> , 2017 , 96,	3.3	2
35	Electron and chemical reservoir corrections for point-defect formation energies. <i>Physical Review B</i> , 2016 , 93,	3.3	42
34	Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 9349-52	3.6	45
33	Mn ₂ V ₂ O ₇ : An Earth Abundant Light Absorber for Solar Water Splitting. <i>Advanced Energy Materials</i> , 2015 , 5, 1401840	21.8	51
32	High optical power and low-efficiency droop blue light-emitting diodes using compositionally step-graded InGa _N barrier. <i>Electronics Letters</i> , 2015 , 51, 1187-1189	1.1	17

31	High Throughput Discovery of Solar Fuels Photoanodes in the CuO/V ₂ O ₅ System. <i>Advanced Energy Materials</i> , 2015 , 5, 1500968	21.8	70
30	First-principles study of electronic structure and photocatalytic properties of MnNiO ₃ as an alkaline oxygen-evolution photocatalyst. <i>Chemical Communications</i> , 2015 , 51, 2867-70	5.8	12
29	Effects of In profile on simulations of InGaN/GaN multi-quantum-well light-emitting diodes. <i>Applied Physics Letters</i> , 2014 , 105, 083507	3.4	24
28	Elastic properties of chemical-vapor-deposited monolayer MoS ₂ , WS ₂ , and their bilayer heterostructures. <i>Nano Letters</i> , 2014 , 14, 5097-103	11.5	384
27	First-principles study of high-field-related electronic behavior of group-III nitrides. <i>Physical Review B</i> , 2014 , 90,	3.3	15
26	First-principles theory of nonradiative carrier capture via multiphonon emission. <i>Physical Review B</i> , 2014 , 90,	3.3	168
25	Effects of strain on the band structure of group-III nitrides. <i>Physical Review B</i> , 2014 , 90,	3.3	73
24	Microscopic origin of the p-type conductivity of the topological crystalline insulator SnTe and the effect of Pb alloying. <i>Physical Review B</i> , 2014 , 89,	3.3	70
23	Origins of optical absorption and emission lines in AlN. <i>Applied Physics Letters</i> , 2014 , 105, 111104	3.4	94
22	Optical polarization characteristics of semipolar (3031) and (3031) InGaN/GaN light-emitting diodes. <i>Optics Express</i> , 2013 , 21 Suppl 1, A53-9	3.3	32
21	Temperature and carrier-density dependence of Auger and radiative recombination in nitride optoelectronic devices. <i>New Journal of Physics</i> , 2013 , 15, 125006	2.9	85
20	Polarization-driven topological insulator transition in a GaN/InN/GaN quantum well. <i>Physical Review Letters</i> , 2012 , 109, 186803	7.4	124
19	Strain effects and band parameters in MgO, ZnO, and CdO. <i>Applied Physics Letters</i> , 2012 , 101, 152105	3.4	56
18	Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes. <i>Applied Physics Letters</i> , 2012 , 101, 231107	3.4	137
17	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. <i>Applied Physics Letters</i> , 2012 , 100, 142110	3.4	107
16	Confinement effects on valence-subband character and polarization anisotropy in (112̄) semipolar InGaN/GaN quantum wells. <i>Journal of Applied Physics</i> , 2012 , 111, 073113	2.5	14
15	Influence of polarity on carrier transport in semipolar (2021̄) and (202̄1) multiple-quantum-well light-emitting diodes. <i>Applied Physics Letters</i> , 2012 , 100, 231110	3.4	48
14	Indium incorporation and emission properties of nonpolar and semipolar InGaN quantum wells. <i>Applied Physics Letters</i> , 2012 , 100, 201108	3.4	148

13	Hybrid functional investigations of band gaps and band alignments for AlN, GaN, InN, and InGaN. <i>Journal of Chemical Physics</i> , 2011 , 134, 084703	3.9	228
12	Influence of Mg-doped barriers on semipolar (202°) multiple-quantum-well green light-emitting diodes. <i>Applied Physics Letters</i> , 2011 , 99, 141114	3.4	18
11	High optical polarization ratio from semipolar (202°) blue-green InGaN/GaN light-emitting diodes. <i>Applied Physics Letters</i> , 2011 , 99, 051109	3.4	67
10	Band parameters and strain effects in ZnO and group-III nitrides. <i>Semiconductor Science and Technology</i> , 2011 , 26, 014037	1.8	48
9	Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. <i>Applied Physics Letters</i> , 2010 , 97, 181102	3.4	29
8	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. <i>Applied Physics Letters</i> , 2009 , 95, 121111	3.4	132
7	Phase diagram of ferroelectric BaTiO ₃ ultrathin films under open-circuit conditions. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 135203	1.8	10
6	Intrinsic current-voltage characteristics of graphene nanoribbon transistors and effect of edge doping. <i>Nano Letters</i> , 2007 , 7, 1469-73	11.5	512
5	Structural and electronic properties of fluorinated double-walled boron nitride nanotubes: Effect of interwall interaction. <i>Physical Review B</i> , 2007 , 75,	3.3	20
4	Making a field effect transistor on a single graphene nanoribbon by selective doping. <i>Applied Physics Letters</i> , 2007 , 91, 253122	3.4	146
3	Mechanism of nanoelectronic switch based on telescoping carbon nanotubes. <i>Applied Physics Letters</i> , 2006 , 88, 173107	3.4	41
2	Ab initio study of transport properties of multiwalled carbon nanotubes. <i>Physical Review B</i> , 2005 , 72,	3.3	46
1	Graph neural network for Hamiltonian-based material property prediction. <i>Neural Computing and Applications</i> , 1	4.8	1