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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.

114 papers	3,171 citations	29 h-index	53 g-index
123 ext. papers	4,159 ext. citations	6.3 avg, IF	5.73 L-index

#	Paper	IF	Citations
114	Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 26560-26568	3.8	314
113	Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS ₂ /AlN(GaN) Heterostructures. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 17594-17599	3.8	269
112	Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. <i>Catalysis Science and Technology</i> , 2017 , 7, 545-559	5.5	251
111	Electronic structures and enhanced optical properties of blue phosphorene/transition metal dichalcogenides van der Waals heterostructures. <i>Scientific Reports</i> , 2016 , 6, 31994	4.9	158
110	Blue Phosphorene/MS ₂ (M = Nb, Ta) Heterostructures As Promising Flexible Anodes for Lithium-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 13449-57	9.5	134
109	Theoretical investigation on the transition-metal borides with Ta ₃ B ₄ -type structure: A class of hard and refractory materials. <i>Computational Materials Science</i> , 2011 , 50, 1559-1566	3.2	121
108	Strain-mediated type-I/type-II transition in MXene/Blue phosphorene van der Waals heterostructures for flexible optical/electronic devices. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 978-984 ^{7.1}	7.1	117
107	Topological insulating in GeTe/Sb ₂ Te ₃ phase-change superlattice. <i>Physical Review Letters</i> , 2012 , 109, 096802	7.4	117
106	Computational mining of photocatalysts for water splitting hydrogen production: two-dimensional InSe-family monolayers. <i>Catalysis Science and Technology</i> , 2017 , 7, 2744-2752	5.5	94
105	Reversible modulation of photoenergy in Sm-doped (K _{0.5} Na _{0.5})NbO ₃ transparent ceramics via photochromic behavior. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 19374-19384	13	59
104	Unexpected elastic isotropy in a black phosphorene/TiC ₂ van der Waals heterostructure with flexible Li-ion battery anode applications. <i>Nano Research</i> , 2017 , 10, 3136-3150	10	55
103	One-pot synthesis of Pt/CeO ₂ /C catalyst for improving the ORR activity and durability of PEMFC. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 13011-13019	6.7	53
102	MOF-Derived Hybrid Hollow Submicrospheres of Nitrogen-Doped Carbon-Encapsulated Bimetallic Ni-Co-S Nanoparticles for Supercapacitors and Lithium Ion Batteries. <i>Inorganic Chemistry</i> , 2019 , 58, 3916-3924 ^{5.1}	5.1	53
101	Band gap engineering in huge-gap semiconductor SrZrO ₃ for visible-light photocatalysis. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 2042-2048	6.7	51
100	The development of two dimensional group IV chalcogenides, blocks for van der Waals heterostructures. <i>Nanoscale</i> , 2016 , 8, 1169-78	7.7	49
99	First-principles investigations of electronic and mechanical properties for stable Ge ₂ Sb ₂ Te ₅ with van der Waals corrections. <i>Computational Materials Science</i> , 2014 , 82, 66-69	3.2	48
98	III-VI van der Waals heterostructures for sustainable energy related applications. <i>Nanoscale</i> , 2019 , 11, 6431-6444	7.7	45

97	Rational construction of heterostructured core-shell Bi ₂ S ₃ @Co ₉ S ₈ complex hollow particles toward high-performance Li- and Na-ion storage. <i>Energy Storage Materials</i> , 2020 , 29, 121-130	19.4	43
96	3D lithiophilic/lithiophobic/lithiophilic dual-gradient porous skeleton for highly stable lithium metal anode. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 313-322	13	43
95	Anion-Anion Mediated Coupling in Layered Perovskite La ₂ Ti ₂ O ₇ for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 13845-13852	3.8	39
94	Electric field-modulated data storage in bilayer InSe. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 12228-12234	7.4	38
93	Role of oxygen vacancies in the resistive switching of SrZrO ₃ for resistance random access memory. <i>Journal of Alloys and Compounds</i> , 2013 , 580, 148-151	5.7	37
92	Pressure-induced topological insulating behavior in the ternary chalcogenide Ge ₂ Sb ₂ Te ₅ . <i>Physical Review B</i> , 2011 , 84,	3.3	35
91	New gallium chalcogenides/arsenene van der Waals heterostructures promising for photocatalytic water splitting. <i>International Journal of Hydrogen Energy</i> , 2018 , 43, 15995-16004	6.7	34
90	Ab initio study of the structure and chemical bonding of stable Ge(3)Sb(2)Te(6). <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 1585-8	3.6	34
89	Origin of p-type conductivity in layered nGeTe/InSb ₂ Te ₃ chalcogenide semiconductors. <i>Physical Review B</i> , 2011 , 83,	3.3	33
88	M ₂ C-type MXenes: Promising catalysts for CO ₂ capture and reduction. <i>Applied Surface Science</i> , 2020 , 521, 146436	6.7	31
87	3D uniform nitrogen-doped carbon skeleton for ultra-stable sodium metal anode. <i>Nano Research</i> , 2020 , 13, 2136-2142	10	30
86	Improving the electrocatalytic properties of Pd-based catalyst for direct alcohol fuel cells: effect of solid solution. <i>Scientific Reports</i> , 2017 , 7, 4907	4.9	30
85	Microstructures and thermodynamic properties of high-entropy alloys CoCrCuFeNi. <i>Intermetallics</i> , 2018 , 93, 40-46	3.5	29
84	In situ boost and reversible modulation of dual-mode photoluminescence under an electric field in a tape-casting-based Er-doped K _{0.5} Na _{0.5} NbO ₃ laminar ceramic. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 7885-7892	7.1	27
83	A Universal Strategy toward the Precise Regulation of Initial Coulombic Efficiency of Li-Rich Mn-Based Cathode Materials. <i>Advanced Materials</i> , 2021 , 33, e2103173	24	27
82	First principles investigation of the structure and electronic properties of Cu ₂ Te. <i>Computational Materials Science</i> , 2014 , 81, 163-169	3.2	26
81	Construction of sugar gourd-like yolk-shell Ni ₃ Mo ₂ CoS ₄ nanocage arrays for high-performance alkaline battery. <i>Energy Storage Materials</i> , 2020 , 25, 105-113	19.4	26
80	Reducing polarization of lithium-sulfur batteries via ZnS/reduced graphene oxide accelerated lithium polysulfide conversion. <i>Materials Today Energy</i> , 2020 , 18, 100519	7	25

79	Few-layer arsenic trichalcogenides: Emerging two-dimensional semiconductors with tunable indirect-direct band-gaps. <i>Journal of Alloys and Compounds</i> , 2017 , 699, 554-560	5.7	23
78	Anchoring Polysulfides and Accelerating Redox Reaction Enabled by Fe-Based Compounds in Lithium Sulfur Batteries. <i>Advanced Functional Materials</i> , 2021 , 31, 2100970	15.6	23
77	Smart white lighting and multi-mode optical modulations via photochromism in Dy-doped KNN-based transparent ceramics. <i>Journal of the American Ceramic Society</i> , 2021 , 104, 903-916	3.8	22
76	The electronic origin of shear-induced direct to indirect gap transition and anisotropy diminution in phosphorene. <i>Nanotechnology</i> , 2015 , 26, 215205	3.4	21
75	First-principles investigations on phase stability and electronic structures of $\text{Yb}_{1-x}\text{M}_x\text{Al}_3$ (M = Ho, Er and Tm) alloys. <i>Intermetallics</i> , 2010 , 18, 2394-2398	3.5	20
74	Strain-induced tunability of optical and photocatalytic properties of ZnO mono-layer nanosheet. <i>Computational Materials Science</i> , 2014 , 91, 38-42	3.2	19
73	Pressure-induced semimetal-semiconductor transition and enhancement of thermoelectric performance in MgAgSb . <i>Applied Physics Letters</i> , 2016 , 108, 213902	3.4	19
72	Defect Management and Multi-Mode Optoelectronic Manipulations via Photo-Thermochromism in Smart Windows. <i>Laser and Photonics Reviews</i> , 2021 , 15, 2100211	8.3	19
71	Manipulating the Local Electronic Structure in Li-Rich Layered Cathode Towards Superior Electrochemical Performance. <i>Advanced Functional Materials</i> , 2021 , 31, 2100783	15.6	16
70	First-principles investigation of mechanical and thermodynamic properties of the rare earth intermetallic YbAl_3 under pressure. <i>Intermetallics</i> , 2012 , 22, 92-98	3.5	15
69	Strain-induced topological insulating behavior in ternary chalcogenide $\text{Ge}_2\text{Sb}_2\text{Te}_5$. <i>Europhysics Letters</i> , 2012 , 97, 27003	1.6	15
68	MXenes: promising donor and acceptor materials for high-efficiency heterostructure solar cells. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 135-143	5.8	15
67	Investigation of the structure and properties of rhombohedral Cu_2Te alloys by ab initio calculations. <i>Intermetallics</i> , 2013 , 32, 292-296	3.5	14
66	Mechanical properties and electronic structure of the incompressible rhenium carbides and nitrides: A first-principles study. <i>Solid State Communications</i> , 2011 , 151, 1842-1845	1.6	14
65	Computational mining of Janus Sc_2C -based MXenes for spintronic, photocatalytic, and solar cell applications. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 10882-10892	13	14
64	Electron interactions and Dirac fermions in graphene- $\text{Ge}_2\text{Sb}_2\text{Te}_5$ superlattices. <i>Journal of Applied Physics</i> , 2014 , 115, 233714	2.5	13
63	Mechanical and bioactive properties of lithium disilicate glass-ceramic mixtures synthesized by two different methods. <i>Journal of Non-Crystalline Solids</i> , 2019 , 509, 1-9	3.9	12
62	First-principle investigation of TcSe_2 monolayer as an efficient visible light photocatalyst for water splitting hydrogen production. <i>Research on Chemical Intermediates</i> , 2017 , 43, 5271-5282	2.8	11

61	Sodiophilic Zn/SnO ₂ porous scaffold to stabilize sodium deposition for sodium metal batteries. <i>Chemical Engineering Journal</i> , 2021 , 404, 126469	14.7	11
60	Piezotronic-enhanced photocatalytic performance of heterostructured BaTiO ₃ /SrTiO ₃ nanofibers. <i>Nano Energy</i> , 2021 , 89, 106391	17.1	11
59	Comprehensive understanding of intrinsic mobility in the monolayers of III-VI group 2D materials. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 21898-21907	3.6	10
58	Elastic Anisotropy and Optic Isotropy in Black Phosphorene/Transition-Metal Trisulfide van der Waals Heterostructures. <i>ACS Omega</i> , 2019 , 4, 4101-4108	3.9	10
57	First-principles investigation on the phase stability and chemical bonding of phase-change random alloys. <i>Solid State Communications</i> , 2010 , 150, 1375-1377	1.6	10
56	Structural and Vibrational Properties of Layered Data Storage Material: Ge ₂ Sb ₂ Te ₅ . <i>Science of Advanced Materials</i> , 2013 , 5, 1493-1497	2.3	10
55	Tunable Contacts in Graphene/InSe van der Waals Heterostructures. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 23699-23706	3.8	10
54	Structural stability and thermoelectric property optimization of Ca ₂ Si. <i>RSC Advances</i> , 2017 , 7, 8936-8943	3.7	9
53	Elastic and thermodynamic properties of the Ti ₂ AlNb orthorhombic phase from first-principles calculations. <i>Physica Status Solidi (B): Basic Research</i> , 2017 , 254, 1600634	1.3	9
52	Manipulating carriers spin polarization in the Heusler alloy Mn ₂ CoAl. <i>RSC Advances</i> , 2015 , 5, 73814-73819	3.7	9
51	Utilizing the different distribution habit of La and Zr in Li-rich Mn-based cathode to achieve fast lithium-ion diffusion kinetics. <i>Journal of Power Sources</i> , 2021 , 499, 229915	8.9	9
50	Layer-Tunable Nonlinear Optical Characteristics and Photocarrier Dynamics of 2D PdSe in Broadband Spectra. <i>Small</i> , 2021 , 17, e2103938	11	8
49	Polyhedral transformation and phase transition in TcO ₂ . <i>RSC Advances</i> , 2015 , 5, 1690-1696	3.7	7
48	Atomic scale insight into the amorphous structure of Cu doped GeTe phase-change material. <i>Journal of Applied Physics</i> , 2014 , 116, 153501	2.5	7
47	Multiscale Deficiency Integration by Na-Rich Engineering for High-Stability Li-Rich Layered Oxide Cathodes. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 8239-8248	9.5	7
46	Prediction of site occupancy of C15 Laves phase at finite temperature based on quasi-harmonic approximation model. <i>Intermetallics</i> , 2018 , 96, 33-40	3.5	6
45	Switchable two-dimensional electrides: A first-principles study. <i>Physical Review B</i> , 2021 , 103,	3.3	6
44	Pressure-induced structure, electronic, thermodynamic and mechanical properties of Ti ₂ AlNb orthorhombic phase by first-principles calculations. <i>Rare Metals</i> , 2021 , 40, 1-11	5.5	6

43	Computational discovery of PtS/GaSe van der Waals heterostructure for solar energy applications. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 20163-20173	3.6	6
42	Breaking the linear scaling relations in MXene catalysts for efficient CO ₂ reduction. <i>Chemical Engineering Journal</i> , 2022 , 429, 132171	14.7	6
41	A lightweight and low-cost electrode for lithium-ion batteries derived from paper towel supported MOF arrays. <i>Chemical Communications</i> , 2020 , 56, 5847-5850	5.8	5
40	The pressure induced twisted distortion in the flexible oxide Tc ₂ O ₇ . <i>CrystEngComm</i> , 2016 , 18, 328-333	3.3	5
39	Boosting Upconversion Photoluminescence and Multielectrical Properties via Er-Doping-Modulated Vacancy Control in BaCaTiZrO. <i>ACS Omega</i> , 2019 , 4, 11004-11013	3.9	5
38	Enhanced photocatalytic performance of black phosphorene by isoelectronic co-dopants. <i>Inorganic Chemistry Frontiers</i> , 2019 , 6, 2369-2378	6.8	5
37	Computational design of double transition metal MXenes with intrinsic magnetic properties.. <i>Nanoscale Horizons</i> , 2022 ,	10.8	5
36	Functionalized Mo ₂ B ₂ MBenes: Promising anchoring and electrocatalysis materials for Lithium-Sulfur battery. <i>Applied Surface Science</i> , 2021 , 566, 150634	6.7	5
35	Ion-conductive gradient sodiophilic 3D scaffold induced homogeneous sodium deposition for highly stable sodium metal batteries. <i>Nano Energy</i> , 2022 , 97, 107202	17.1	5
34	Effect of nickel doping on structure and suppressing boron volatility of borosilicate glass sealants in solid oxide fuel cells. <i>Journal of the European Ceramic Society</i> , 2019 , 39, 2179-2185	6	4
33	Structural transformation-induced surface strengthening of borosilicate sealing glass for solid oxide fuel cells. <i>Ceramics International</i> , 2019 , 45, 15629-15635	5.1	4
32	Electronic Anisotropy and Superconductivity in One-Dimensional Electride Ca ₃ Si. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7683-7690	3.8	4
31	Different topological insulating behavior in E ₁ GaS and GaS-II under uniaxial tension. <i>Physical Review B</i> , 2013 , 88,	3.3	4
30	Electronic mechanism of shear modulus enhancement in rare earth intermetallics Yb _{1-x} Tm _x Al ₃ . <i>Intermetallics</i> , 2011 , 19, 1020-1023	3.5	4
29	Investigation on Ge _{5-x} Sb _x Te ₅ phase-change materials by first-principles method. <i>Applied Physics A: Materials Science and Processing</i> , 2010 , 99, 961-964	2.6	4
28	Prediction of superconductivity and topological aspects in single-layer Bi ₂ Pd. <i>Physical Review B</i> , 2020 , 102,	3.3	4
27	InSe/Te van der Waals Heterostructure as a High-Efficiency Solar Cell from Computational Screening. <i>Materials</i> , 2021 , 14,	3.5	4
26	Rapid and Large-Scale Quality Assessment of Two-Dimensional MoS ₂ Using Sulfur Particles with Optical Visualization. <i>Nano Letters</i> , 2021 , 21, 1260-1266	11.5	4

25	High-performance III-VI monolayer transistors for flexible devices. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 7039-7047	3.6	3
24	Rigid-resilient transition in calcium borosilicate sealing glass/ceramics: Effect of preferred orientation. <i>Journal of the European Ceramic Society</i> , 2018 , 38, 2410-2416	6	3
23	Structural behavior and in vitro bioactivity evaluation of hydroxyapatite-like bioactive glass based on the SiO ₂ -CaO-P ₂ O ₅ system. <i>Ceramics International</i> , 2021 , 47, 18094-18104	5.1	3
22	Simultaneously achieving high performance of energy storage and transparency via A-site non-stoichiometric defect engineering in KNN-based ceramics. <i>Chemical Engineering Journal</i> , 2022 , 444, 136538	14.7	3
21	Two-dimensional O-phase group III monochalcogenides for photocatalytic water splitting. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 065501	1.8	2
20	Local atomic structure in molten Si ₃ Sb ₂ Te ₃ phase change material. <i>Solid State Communications</i> , 2012 , 152, 100-103	1.6	2
19	Phase stability and electronic structure of Si ₂ Sb ₂ Te ₅ phase-change material. <i>Journal of Physics and Chemistry of Solids</i> , 2010 , 71, 1165-1167	3.9	2
18	The Electronic Origin of the Underestimated Trigonal Shear Constant of Zr _{1-x} Nb _x Super Alloys from First-Principles Calculations. <i>Science of Advanced Materials</i> , 2014 , 6, 659-664	2.3	2
17	The interlayer coupling modulation of a g-CN/WTe heterostructure for solar cell applications.. <i>RSC Advances</i> , 2021 , 12, 998-1004	3.7	2
16	Effect of nitrogen on the structure evolution and biological properties of mesoporous bioactive glass nanospheres: Experiments and simulations. <i>Journal of Non-Crystalline Solids</i> , 2022 , 578, 121329	3.9	2
15	Two-dimensional (Zr _{0.5} Hf _{0.5}) ₂ CO ₂ : A promising visible light water-splitting photocatalyst with efficiently carrier separation. <i>Computational Materials Science</i> , 2021 , 186, 110013	3.2	2
14	Computational mining of the pressure effect on thermodynamic and thermoelectric properties of cubic Ca ₂ Si. <i>Europhysics Letters</i> , 2018 , 123, 67003	1.6	2
13	Enhancing cycling stability in Li-rich Mn-based cathode materials by solid-liquid-gas integrated interface engineering. <i>Nano Energy</i> , 2022 , 97, 107201	17.1	2
12	Pressure-Induced Destabilization and Anomalous Lattice Distortion in TcO. <i>Inorganic Chemistry</i> , 2017 , 56, 9973-9978	5.1	1
11	Ab Initio Study on Hexagonal Ge ₂ Sb ₂ Te ₅ -A Phase-Change Material for Nonvolatile Memories. <i>Materials Science Forum</i> , 2011 , 687, 7-11	0.4	1
10	GeP/NbX (X=S, Se) Nano-Heterostructures: Promising Isotropic Flexible Anodes for Lithium-Ion Batteries with High Lithium Storage Capacity. <i>ACS Omega</i> , 2021 , 6, 2956-2965	3.9	1
9	Effect of B ₂ O ₃ on the structural and in vitro biological assessment of mesoporous bioactive glass nanospheres. <i>Journal of the American Ceramic Society</i> , 2021 , 104, 3058-3072	3.8	1
8	Understanding the anchoring effect on Li plating with Indium Tin oxide layer functionalized hosts for Li metal anodes. <i>Chemical Engineering Journal</i> , 2022 , 440, 135827	14.7	1

7	Atomically scale design of van der Waals heterostructures as photocatalysts 2020 , 511-525		o
6	Promoting effect of (Co, Ni)O solid solution on Pd catalysts for ethylene glycol electrooxidation in alkaline solution. <i>Electrochimica Acta</i> , 2022 , 408, 139965	6.7	o
5	Structural, Electronic, and Nonlinear Optical Properties of CH and CCl Encapsulating Li and F Atoms. <i>ACS Omega</i> , 2021 , 6, 16234-16240	3.9	o
4	Microscopic origin of graphene nanosheets derived from coal-tar pitch by treating ALC as the intermediate. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 12449-12455	3.6	o
3	A reasonable approach to describe the atom distributions and configurational entropy in high entropy alloys based on site preference. <i>Intermetallics</i> , 2022 , 144, 107489	3.5	o
2	Hybrid Chiral MoS Layers for Spin-Polarized Charge Transport and Spin-Dependent Electrocatalytic Applications.. <i>Advanced Science</i> , 2022 , e2201063	13.6	o
1	Tailoring micro-structure of eco-friendly temperature-insensitive transparent ceramics achieving superior piezoelectricity. <i>Acta Materialia</i> , 2022 , 118061	8.4	o