Eâ€j Kan

List of Publications by Year
in descending order

160 papers	8,300 citations	53660 45 h-index	51492 86 g-index
165 all docs	165 docs citations	165 times ranked	9402 citing authors

#	Article	IF	Citations
1	Semiconducting Groupâ€...15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie - International Edition, 2016, 55, 1666-1669.	7.2	651
2	Half-Metallicity in Edge-Modified Zigzag Graphene Nanoribbons. Journal of the American Chemical Society, 2008, 130, 4224-4225.	6.6	640
3	Semiconducting Groupâ€...15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. Angewandte Chemie, 2016, 128, 1698-1701.	1.6	315
4	Will zigzag graphene nanoribbon turn to half metal under electric field?. Applied Physics Letters, 2007, 91, .	1.5	299
5	Toward Intrinsic Room-Temperature Ferromagnetism in Two-Dimensional Semiconductors. Journal of the American Chemical Society, 2018, 140, 11519-11525.	6.6	280
6	Predicting the spin-lattice order of frustrated systems from first principles. Physical Review B, 2011, 84, .	1.1	262
7	Prediction of Intrinsic Ferromagnetic Ferroelectricity in a Transition-Metal Halide Monolayer. Physical Review Letters, 2018, 120, 147601.	2.9	217
8	MnO2 Nanorods Intercalating Graphene Oxide/Polyaniline Ternary Composites for Robust High-Performance Supercapacitors. Scientific Reports, 2014, 4, 4824.	1.6	215
9	Stabilization of the Metastable Lead Iodide Perovskite Phase via Surface Functionalization. Nano Letters, 2017, 17, 4405-4414.	4.5	204
10	Tunable Magnetism in a Nonmetal-Substituted ZnO Monolayer: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 11336-11342.	1.5	180
11	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. Nano Letters, 2015, 15, 8277-8281.	4.5	168
12	Visible-Light-Absorption in Graphitic C₃N₄ Bilayer: Enhanced by Interlayer Coupling. Journal of Physical Chemistry Letters, 2012, 3, 3330-3334.	2.1	138
13	Towards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approach. Physical Review Letters, 2013, 110, 118702.	2.9	136
14	Half-metallicity in hybrid BCN nanoribbons. Journal of Chemical Physics, 2008, 129, 084712.	1.2	133
15	â€œNarrowâ€•Graphene Nanoribbons Made Easier by Partial Hydrogenation. Nano Letters, 2009, 9, 4025-4030.	4.5	120
16	Sandwich-structured MnO₂/polypyrrole/reduced graphene oxide hybrid composites for high-performance supercapacitors. RSC Advances, 2014, 4, 9898-9904.	1.7	113
17	Quantum anomalous Hall effect in ferromagnetic transition metal halides. Physical Review B, 2017, 95, .	1.1	110
18	Cobalt Sulfide/Graphene Composite Hydrogel as Electrode for High-Performance Pseudocapacitors. Scientific Reports, 2016, 6, 21717.	1.6	105

#	Article	IF	Citations
19	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2012, 116, 3142-3146.	1.5	103
20	Half-Metallicity in Organic Single Porous Sheets. Journal of the American Chemical Society, 2012, 134, 5718-5721.	6.6	101
21	General Theory for the Ferroelectric Polarization Induced by Spin-Spiral Order. Physical Review Letters, 2011, 107, 157202.	2.9	100
22	Boron-substituted graphyne as a versatile material with high storage capacities of Li and H2: a multiscale theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 16120.	1.3	96
23	Theoretical Prediction of Phosphorene and Nanoribbons As Fast-Charging Li Ion Battery Anode Materials. Journal of Physical Chemistry C, 2015, 119, 6923-6928.	1.5	96
24	Van der Waals bilayer antimonene: A promising thermophotovoltaic cell material with 31% energy conversion efficiency. Nano Energy, 2017, 38, 561-568.	8.2	92
25	Switchable encapsulation of polysulfides in the transition between sulfur and lithium sulfide. Nature Communications, 2020, 11, 845.	5.8	92
26	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. Physical Review Letters, 2020, 124, 067602.	2.9	84
27	Substitutionally Dispersed Highâ€Oxidation CoO<i>_x</i> Clusters in the Lattice of Rutile TiO₂ Triggering Efficient Coï£¿Ti Cooperative Catalytic Centers for Oxygen Evolution Reactions. Advanced Functional Materials, 2021, 31, 2009610.	7.8	82
28	High-Temperature Ferromagnetism in an Fe₃P Monolayer with a Large Magnetic Anisotropy. Journal of Physical Chemistry Letters, 2019, 10, 2733-2738.	2.1	79
29	The Janus structures of group-III chalcogenide monolayers as promising photocatalysts for water splitting. Applied Surface Science, 2019, 478, 522-531.	3.1	78
30	Prominently Improved Hydrogen Purification and Dispersive Metal Binding for Hydrogen Storage by Substitutional Doping in Porous Graphene. Journal of Physical Chemistry C, 2012, 116, 21291-21296.	1.5	76
31	Boosting the Curie Temperature of Two-Dimensional Semiconducting CrI₃ Monolayer through van der Waals Heterostructures. Journal of Physical Chemistry C, 2019, 123, 17987-17993.	1.5	74
32	MAGNETISM IN GRAPHENE SYSTEMS. Nano, 2008, 03, 433-442.	0.5	70
33	Accurate K-edge X-ray photoelectron and absorption spectra of g-C₃N₄ nanosheets by first-principles simulations and reinterpretations. Physical Chemistry Chemical Physics, 2019, 21, 22819-22830.	1.3	70
34	Lithium-doped MOF impregnated with lithium-coated fullerenes: A hydrogen storage route for high gravimetric and volumetric uptakes at ambient temperatures. Chemical Communications, 2011, 47, 7698.	2.2	60
35	Water-sprouted, plasma-enhanced Ni-Co phospho-nitride nanosheets boost electrocatalytic hydrogen and oxygen evolution. Chemical Engineering Journal, 2020, 402, 126257.	6.6	60
36	Two-Dimensional Hexagonal Transition-Metal Oxide for Spintronics. Journal of Physical Chemistry Letters, 2013, 4, 1120-1125.	2.1	58

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37	Ultrathin molybdenum disulfide/carbon nitride nanosheets with abundant active sites for enhanced hydrogen evolution. Nanoscale, 2018, 10, 1766-1773.	2.8	57
38	Half-Metallic Ferromagnetism and Large Negative Magnetoresistance in the New Lacunar Spinel GaTi₃VS₈. Journal of the American Chemical Society, 2010, 132, 5704-5710.	6.6	55
39	New Ferroelectric Phase in Atomic-Thick Phosphorene Nanoribbons: Existence of in-Plane Electric Polarization. Nano Letters, 2016, 16, 8015-8020.	4.5	55
40	Efficient Carrier Separation and Band Structure Tuning of Two-Dimensional C₂N/GaTe van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 15892-15902.	1.5	55
41	Prediction for room-temperature half-metallic ferromagnetism in the half-fluorinated single layers of BN and ZnO. Applied Physics Letters, 2010, 97, .	1.5	54
42	Progress and prospects in lowâ€dimensional multiferroic materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1409.	6.2	53
43	Room-Temperature Ferroelectricity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:msup><mml:mrow><mml:mi mathvariant="normal">T</mml:mi></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></mml:mrow></mml:msup></mml:mrow></m - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>ReS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m Multilayers. Physical Review Letters, 2022, 128, 067601.	2.9	52
44	A promising monolayer membrane for oxygen separation from harmful gases: nitrogen-substituted polyphenylene. Nanoscale, 2014, 6, 9960-9964.	2.8	51
45	Electronic and magnetic properties of an AlN monolayer doped with first-row elements: a first-principles study. RSC Advances, 2015, 5, 18352-18358.	1.7	50
46	Thermodynamically stable single-side hydrogenated graphene. Physical Review B, 2010, 82, .	1.1	47
47	Ru Colloidosome Catalysts for the Hydrogen Oxidation Reaction in Alkaline Media. Journal of the American Chemical Society, 2022, 144, 11138-11147.	6.6	47
48	Ultra-High-Temperature Ferromagnetism in Intrinsic Tetrahedral Semiconductors. Journal of the American Chemical Society, 2019, 141, 12413-12418.	6.6	44
49	Magnetic states of zigzag graphene nanoribbons from first principles. Applied Physics Letters, 2009, 94, .	1.5	41
50	Theoretical understanding of magnetic and electronic structures of Ti3C2 monolayer and its derivatives. Solid State Communications, 2015, 222, 9-13.	0.9	41
51	Electride: from computational characterization to theoretical design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 430-440.	6.2	41
52	Electron-induced ferromagnetic ordering of Co-doped ZnO. Journal of Applied Physics, 2007, 102, 033915.	1.1	40
53	Stabilizing intrinsic defects in SnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	1.1	40
54	Mechanical, Electronic, and Magnetic Properties of NiX₂ (X = Cl, Br, I) Layers. ACS Omega, 2019, 4, 5714-5721.	1.6	40

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55	Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. Applied Physics Letters, 2010, 96, .	1.5	39
56	Single-ion anisotropy, Dzyaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mfrac><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mi xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>R</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mm Physical Review B, 2011, 83, .	1.1	39
57	Improved permeability and selectivity in porous graphene for hydrogen purification. Physical Chemistry Chemical Physics, 2014, 16, 25755-25759.	1.3	39
58	Theoretical Analysis of the Spin Exchange and Magnetic Dipoleâ˜'Dipole Interactions Leading to the Magnetic Structure of Ni₃TeO₆. Inorganic Chemistry, 2010, 49, 7545-7548.	1.9	38
59	Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 17252-17254.	1.5	38
60	Prediction of room-temperature ferromagnetism in a two-dimensional direct band gap semiconductor. Nanoscale, 2020, 12, 15670-15676.	2.8	38
61	Catenated metal-organic frameworks: Promising hydrogen purification materials and high hydrogen storage medium with further lithium doping. International Journal of Hydrogen Energy, 2013, 38, 9811-9818.	3.8	37
62	Electronic structure of atomic Ti chains on semiconducting graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2007, 127, 164706.	1.2	34
63	Superhalogens as building blocks of two-dimensional organicâ€"inorganic hybrid perovskites for optoelectronics applications. Nanoscale, 2016, 8, 17836-17842.	2.8	34
64	Electronic properties and hydrogen storage application of designed porous nanotubes from a polyphenylene network. International Journal of Hydrogen Energy, 2014, 39, 18966-18975.	3.8	33
65	Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator. Journal of Physical Chemistry Letters, 2016, 7, 1919-1924.	2.1	33
66	First-Principles Prediction of Room-Temperature Ferromagnetic Semiconductor MnS₂ via Isovalent Alloying. Journal of Physical Chemistry C, 2019, 123, 10114-10119.	1.5	33
67	Origin of the Ising ferrimagnetism and spin-charge coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LuFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml: Physical Review B, 2009, 80, .	1.1	32
68	Prediction of another semimetallic silicene allotrope with Dirac fermions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 3754-3759.	0.9	31
69	Giant Biquadratic Exchange in 2D Magnets and Its Role in Stabilizing Ferromagnetism of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NiCl</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn>< Monolayers. Physical Review Letters, 2021, 127, 247204.	2.9	31
70	High-temperature ferro-electricity in two-dimensional atomic crystal. Applied Physics Letters, 2013, 103, .	1.5	30
71	Discovery of twin orbital-order phases in ferromagnetic semiconducting VI₃ monolayer. Physical Chemistry Chemical Physics, 2020, 22, 512-517.	1.3	29
72	Density-functional analysis of spin exchange and ferroelectric polarization in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>AgCrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml: Physical Review B, 2009, 80, .	1.1	28

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73	Orbital order and partial electronic delocalization in a triangular magnetic metal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ag</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 81, .	1.1	28
74	A promising two-dimensional channel material: monolayer antimonide phosphorus. Science China Materials, 2016, 59, 648-656.	3.5	28
75	Theoretical Investigation of the Magnetic Structure and Ferroelectric Polarization of the Multiferroic Langasite Ba₃NbFe₃Si₂O₁₄. Chemistry of Materials, 2010, 22, 5290-5295.	3.2	26
76	Density Functional Theory Analysis of the Interplay between Jahnâˆ'Teller Instability, Uniaxial Magnetism, Spin Arrangement, Metalâˆ'Metal Interaction, and Spinâˆ'Orbit Coupling in Ca₃CoMO₆ (M = Co, Rh, Ir). Inorganic Chemistry, 2011, 50, 1758-1766.	1.9	25
77	Graphene Nanoribbons: Geometric, Electronic, and Magnetic Properties. , 0, , .		25
78	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, .	3.9	25
79	Toward Room-Temperature Electrical Control of Magnetic Order in Multiferroic van der Waals Materials. Nano Letters, 2022, 22, 5191-5197.	4.5	25
80	Two-dimensional organometallic porous sheets with possible high-temperature ferromagnetism. Nanoscale, 2012, 4, 5304.	2.8	23
81	Biaxial strain effect on the electronic and magnetic phase transitions in double perovskite La2FeMnO6: A first-principles study. Journal of Applied Physics, 2013, 114, .	1.1	23
82	Ferroelectricity in Perovskites with s⁰ Aâ€Site Cations: Toward Nearâ€Roomâ€Temperature Multiferroics. Angewandte Chemie - International Edition, 2010, 49, 1603-1606.	7.2	22
83	Ï€-Back-Donation Effect of the Cyanide Ligands on the Electron Correlation and Charge Transfer in Prussian Blue RbMn[Fe(CN)₆]. Inorganic Chemistry, 2010, 49, 3086-3088.	1.9	22
84	The effect of oxygen vacancy on the half-metallic nature of double perovskite Sr2FeMoO6: A theoretical study. Solid State Communications, 2014, 177, 57-60.	0.9	22
85	Enhancing magnetic vacancies in semiconductors by strain. Applied Physics Letters, 2012, 100, 072401.	1.5	21
86	The effect of biaxial mechanical strain on the physical properties of double perovskite Sr2FeMoO6: A theoretical study. Solid State Communications, 2014, 191, 70-75.	0.9	21
87	High-capacity hydrogen storage in Li-adsorbed g-C3N4. Materials Chemistry and Physics, 2016, 180, 440-444.	2.0	21
88	Designing half-metallic ferromagnetism by a new strategy: an example of superhalogen modified graphitic C₃N₄. Journal of Materials Chemistry C, 2018, 6, 1709-1714.	2.7	21
89	Controllable vdW Contacts between the Ferroelectric In₂Se₃ Monolayer and Two-Dimensional Metals. Journal of Physical Chemistry C, 2021, 125, 10738-10746.	1.5	21
90	Trimetallic Octahedral Niâ€"Coâ€"W Phosphoxide Sprouted from Plasma-Defect-Engineered Niâ€"Co Support for Ultrahigh-Performance Electrocatalytic Hydrogen Evolution. ACS Sustainable Chemistry and Engineering, 2021, 9, 7454-7465.	3.2	21

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91	Tunable band gap and hydrogen adsorption property of a two-dimensional porous polymer by nitrogen substitution. Physical Chemistry Chemical Physics, 2013, 15, 666-670.	1.3	20
92	Tuning Electronic and Magnetic Properties of Two-Dimensional Ferromagnetic Semiconductor CrI₃ through Adsorption of Benzene. Journal of Physical Chemistry C, 2020, 124, 22143-22149.	1.5	20
93	First-principles study of interaction between H2 molecules and BN nanotubes with BN divacancies. Journal of Chemical Physics, 2007, 127, 164718.	1.2	19
94	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. Solid State Communications, 2011, 151, 1228-1230.	0.9	19
95	Spin Reorientation in the Square-Lattice Antiferromagnets RMnAsO (R = Ce, Nd): Density Functional Analysis of the Spin-Exchange Interactions between the Rare-Earth and Transition-Metal Ions. Inorganic Chemistry, 2012, 51, 6890-6897.	1.9	19
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98	Built-in electric field control of magnetic coupling in van der Waals semiconductors. Physical Review B, 2021, 103, .	1.1	19
99	Popcorn-like Co₃O₄ nanoparticles confined in a three-dimensional hierarchical N-doped carbon nanotube network as a highly-efficient trifunctional electrocatalyst for zincâ€“air batteries and water splitting devices. Inorganic Chemistry Frontiers, 2022, 9, 2517-2529.	3.0	18
100	Unzipping carbon nanotubes into nanoribbons upon oxidation: A first-principles study. Nanoscale, 2012, 4, 1254.	2.8	17
101	Tunable ferroelectric single-atom catalysis of CO oxidation using a Pt/In₂Se₃ monolayer. Journal of Materials Chemistry A, 2020, 8, 20725-20731.	5.2	17
102	Analysis of the Magnetic Structure and Ferroelectric Polarization of Monoclinic MnSb2S4by Density Functional Theory Calculations. Inorganic Chemistry, 2010, 49, 10956-10959.	1.9	16
103	Geometric and Electronic Structures as well as Thermodynamic Stability of Hexyl-Modified Silicon Nanosheet. Journal of Physical Chemistry C, 2013, 117, 13283-13288.	1.5	16
104	Will a graphitic-like ZnO single-layer be an ideal substrate for graphene?. RSC Advances, 2014, 4, 17478.	1.7	16
105	The layered ferromagnet Cs2AgF4: Antiferromagnetic inter-layer coupling driven by magnetic dipole-dipole interactions. Zeitschrift FÃ¼r Kristallographie, 2010, 225, .	1.1	15
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107	First-principles calculations of the electronic and magnetic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cs</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Ag</mml:mi><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	1.1	14
108	Enabling High Loading in Singleâ€Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites. Small, 2022, 18, e2200073.	5.2	14

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109	A Bâ€“Câ€“N hybrid porous sheet: an efficient metal-free visible-light absorption material. Physical Chemistry Chemical Physics, 2014, 16, 4299.	1.3	13
110	A promising way to open an energy gap in bilayer graphene. Nanoscale, 2015, 7, 17096-17101.	2.8	13
111	Computational Dissection of 2D SiC₇ Monolayer: A Direct Band Gap Semiconductor and High Power Conversion Efficiency. Advanced Theory and Simulations, 2019, 2, 1900058.	1.3	13
112	On the Importance of the Interplaquette Spin Exchanges in Na₃RuO₄: Density Functional Theory Analysis of the Spin Exchange and Magnetic Properties. Inorganic Chemistry, 2010, 49, 3025-3028.	1.9	12
113	Influences of lithium doping and fullerene impregnation on hydrogen storage in metal organic frameworks. Molecular Simulation, 2013, 39, 968-974.	0.9	12
114	Edge-Modified Graphene Nanoribbons: Appearance of Robust Spiral Magnetism. Journal of Physical Chemistry C, 2017, 121, 1371-1376.	1.5	12
115	Nature of spin-lattice coupling in two-dimensional CrI3 and CrGeTe3. Science China: Physics, Mechanics and Astronomy, 2021, 64, 1.	2.0	12
116	Graphene-mediated ferromagnetic coupling in the nickel nano-islands/graphene hybrid. Science Advances, 2021, 7, .	4.7	12
117	Electrical rectification by selective wave-function coupling in small Ag clusters on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>111</mml:m Physical Review B, 2010, 81, .	1.1	11
118	On the High Magnetic-Ordering Temperature of the 5d Magnetic Oxide Ca₃LiOsO₆ Crystallizing in a Trigonal Crystal Structure: Density Functional Analysis. Inorganic Chemistry, 2011, 50, 4182-4186.	1.9	11
119	Stability of graphitic-like zinc oxide layers under carriers doping: a first-principles study. Nanoscale, 2013, 5, 12111.	2.8	10
120	d0 magnetism in semiconductors through confining delocalized atomic orbitals. Applied Physics Letters, 2013, 102, 022422.	1.5	10
121	Two-dimensional silicon monolayers generated on c-BN(111) substrate. Physical Chemistry Chemical Physics, 2015, 17, 15694-15700.	1.3	10
122	Half-metallicity obtained in silicene nanosheet by nitrogenation engineering. Journal of Applied Physics, 2016, 120, 234303.	1.1	9
123	Two-dimensional metal-free boron chalcogenides B₂X₃ (X = Se and Te) as photocatalysts for water splitting under visible light. Nanoscale, 2021, 13, 3627-3632.	2.8	9
124	High-Temperature p-Orbital Half-Metallicity and Out-of-Plane Piezoelectricity in a GaN Monolayer Induced by Superhalogens. Journal of Physical Chemistry C, 2021, 125, 10027-10033.	1.5	9
125	Density Functional Investigation of the Difference in the Magnetic Structures of the Layered Triangular Antiferromagnets CuFeO2and AgCrO2. Chemistry of Materials, 2011, 23, 4181-4185.	3.2	8
126	Vacancy-induced insulator â€“ direct spin gapless semiconductor â€“ half-metal transition in double perovskite La2CrFeO6: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 2897-2901.	0.9	8

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128	Selective Construction of Magic Hierarchical Metalâ€“Organic Clusters on Surfaces. Journal of Physical Chemistry C, 2021, 125, 358-365.	1.5	8
129	High-throughput calculations of spintronic tetra-phase transition metal dinitrides. Journal of Materials Chemistry C, 2021, 9, 14401-14407.	2.7	8
130	Carrier-tunable magnetism of graphene with single-atom vacancy. Journal of Applied Physics, 2013, 113, 213709.	1.1	7
131	Ferroelectric-like structural transition in metallic LiOsO3. RSC Advances, 2014, 4, 26843.	1.7	7
132	Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance. Physical Review B, 2016, 94, .	1.1	7
133	Unconventional distortion induced two-dimensional multiferroicity in a CrO₃ monolayer. Nanoscale, 2021, 13, 13048-13056.	2.8	7
134	First-principles investigations on the magnetic structure of Î±-NaMnO₂. Journal of Physics Condensed Matter, 2012, 24, 456002.	0.7	5
135	Atomically dispersed tungsten on metal halide monolayer as a ferromagnetic Chern insulator. Physical Review B, 2018, 98, .	1.1	5
136	Hexagonal Boron Nitrideâ€“Metal Junction: Removing the Schottky Barriers by Grain Boundary. Advanced Theory and Simulations, 2018, 1, 1800045.	1.3	5
137	Atomically thin mononitrides SiN and GeN: New two-dimensional wide band gap semiconductors. Europhysics Letters, 2018, 122, 47002.	0.7	5
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139	Theoretical study of CO oxidation on cationic, neutral, and anionic AuM dimers (M = Pd and Ag). Journal of Molecular Modeling, 2014, 20, 2313.	0.8	4
140	Theoretical realization of half-metallicity in two-dimensional monolayered molybdenum dinitride by Mo vacancy tuning. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2669-2673.	0.9	4
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