

# E j Kan

## List of Publications by Citations

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7,301  
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#	Paper	IF	Citations
157	Half-metallicity in edge-modified zigzag graphene nanoribbons. <i>Journal of the American Chemical Society</i> , <b>2008</b> , 130, 4224-5	16.4	587
156	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 1666-9	16.4	535
155	Will zigzag graphene nanoribbon turn to half metal under electric field?. <i>Applied Physics Letters</i> , <b>2007</b> , 91, 243116	3.4	285
154	Semiconducting Group 15 Monolayers: A Broad Range of Band Gaps and High Carrier Mobilities. <i>Angewandte Chemie</i> , <b>2016</b> , 128, 1698-1701	3.6	254
153	MnO <sub>2</sub> nanorods intercalating graphene oxide/polyaniline ternary composites for robust high-performance supercapacitors. <i>Scientific Reports</i> , <b>2014</b> , 4, 4824	4.9	176
152	Toward Intrinsic Room-Temperature Ferromagnetism in Two-Dimensional Semiconductors. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 11519-11525	16.4	170
151	Predicting the spin-lattice order of frustrated systems from first principles. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	166
150	Stabilization of the Metastable Lead Iodide Perovskite Phase via Surface Functionalization. <i>Nano Letters</i> , <b>2017</b> , 17, 4405-4414	11.5	151
149	. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 11336-11342	3.8	150
148	Prediction of Intrinsic Ferromagnetic Ferroelectricity in a Transition-Metal Halide Monolayer. <i>Physical Review Letters</i> , <b>2018</b> , 120, 147601	7.4	149
147	Atomically Thin Transition-Metal Dinitrides: High-Temperature Ferromagnetism and Half-Metallicity. <i>Nano Letters</i> , <b>2015</b> , 15, 8277-81	11.5	132
146	Half-metallicity in hybrid BCN nanoribbons. <i>Journal of Chemical Physics</i> , <b>2008</b> , 129, 084712	3.9	129
145	Visible-Light-Absorption in Graphitic C <sub>3</sub> N <sub>4</sub> Bilayer: Enhanced by Interlayer Coupling. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 3330-3334	6.4	123
144	"Narrow" graphene nanoribbons made easier by partial hydrogenation. <i>Nano Letters</i> , <b>2009</b> , 9, 4025-30	11.5	115
143	Towards direct-gap silicon phases by the inverse band structure design approach. <i>Physical Review Letters</i> , <b>2013</b> , 110, 118702	7.4	112
142	Sandwich-structured MnO <sub>2</sub> /polypyrrole/reduced graphene oxide hybrid composites for high-performance supercapacitors. <i>RSC Advances</i> , <b>2014</b> , 4, 9898-9904	3.7	101
141	Cobalt Sulfide/Graphene Composite Hydrogel as Electrode for High-Performance Pseudocapacitors. <i>Scientific Reports</i> , <b>2016</b> , 6, 21717	4.9	91

140	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 3142-3146	3.8	88
139	Half-metallicity in organic single porous sheets. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 5718-5721	6.4	87
138	Theoretical Prediction of Phosphorene and Nanoribbons As Fast-Charging Li Ion Battery Anode Materials. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 6923-6928	3.8	83
137	General theory for the ferroelectric polarization induced by spin-spiral order. <i>Physical Review Letters</i> , <b>2011</b> , 107, 157202	7.4	81
136	Van der Waals bilayer antimonene: A promising thermophotovoltaic cell material with 31% energy conversion efficiency. <i>Nano Energy</i> , <b>2017</b> , 38, 561-568	17.1	78
135	Boron-substituted graphyne as a versatile material with high storage capacities of Li and H <sub>2</sub> : a multiscale theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 16120-6	3.6	78
134	Quantum anomalous Hall effect in ferromagnetic transition metal halides. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	69
133	Prominently Improved Hydrogen Purification and Dispersive Metal Binding for Hydrogen Storage by Substitutional Doping in Porous Graphene. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 21291-21296	3.8	68
132	MAGNETISM IN GRAPHENE SYSTEMS. <i>Nano</i> , <b>2008</b> , 03, 433-442	1.1	61
131	Lithium-doped MOF impregnated with lithium-coated fullerenes: a hydrogen storage route for high gravimetric and volumetric uptakes at ambient temperatures. <i>Chemical Communications</i> , <b>2011</b> , 47, 7698-7700	5.8	53
130	Switchable encapsulation of polysulfides in the transition between sulfur and lithium sulfide. <i>Nature Communications</i> , <b>2020</b> , 11, 845	17.4	51
129	High-Temperature Ferromagnetism in an FeP Monolayer with a Large Magnetic Anisotropy. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2733-2738	6.4	50
128	Two-Dimensional Hexagonal Transition-Metal Oxide for Spintronics. <i>Journal of Physical Chemistry Letters</i> , <b>2013</b> , 4, 1120-5	6.4	49
127	A promising monolayer membrane for oxygen separation from harmful gases: nitrogen-substituted polyphenylene. <i>Nanoscale</i> , <b>2014</b> , 6, 9960-4	7.7	47
126	Ultrathin molybdenum disulfide/carbon nitride nanosheets with abundant active sites for enhanced hydrogen evolution. <i>Nanoscale</i> , <b>2018</b> , 10, 1766-1773	7.7	46
125	New Ferroelectric Phase in Atomic-Thick Phosphorene Nanoribbons: Existence of in-Plane Electric Polarization. <i>Nano Letters</i> , <b>2016</b> , 16, 8015-8020	11.5	46
124	Half-metallic ferromagnetism and large negative magnetoresistance in the new lacunar spinel GaTi <sub>3</sub> VS <sub>8</sub> . <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 5704-10	16.4	46
123	Prediction for room-temperature half-metallic ferromagnetism in the half-fluorinated single layers of BN and ZnO. <i>Applied Physics Letters</i> , <b>2010</b> , 97, 122503	3.4	45

122	Thermodynamically stable single-side hydrogenated graphene. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	44
121	The Janus structures of group-III chalcogenide monolayers as promising photocatalysts for water splitting. <i>Applied Surface Science</i> , <b>2019</b> , 478, 522-531	6.7	40
120	Electron-induced ferromagnetic ordering of Co-doped ZnO. <i>Journal of Applied Physics</i> , <b>2007</b> , 102, 033915.	5.5	39
119	Electrical Control of Magnetic Phase Transition in a Type-I Multiferroic Double-Metal Trihalide Monolayer. <i>Physical Review Letters</i> , <b>2020</b> , 124, 067602	7.4	38
118	Boosting the Curie Temperature of Two-Dimensional Semiconducting CrI <sub>3</sub> Monolayer through van der Waals Heterostructures. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 17987-17993	3.8	38
117	Stabilizing intrinsic defects in SnO <sub>2</sub> . <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	38
116	Substitutionally Dispersed High-Oxidation CoO <sub>x</sub> Clusters in the Lattice of Rutile TiO <sub>2</sub> Triggering Efficient Co/Ti Cooperative Catalytic Centers for Oxygen Evolution Reactions. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2009610	15.6	38
115	Electronic and magnetic properties of an AlN monolayer doped with first-row elements: a first-principles study. <i>RSC Advances</i> , <b>2015</b> , 5, 18352-18358	3.7	37
114	Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. <i>Applied Physics Letters</i> , <b>2010</b> , 96, 102503	3.4	37
113	Magnetic states of zigzag graphene nanoribbons from first principles. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 223105	3.4	37
112	Improved permeability and selectivity in porous graphene for hydrogen purification. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 25755-9	3.6	35
111	Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 17252-17254	3.8	35
110	Catenated metal-organic frameworks: Promising hydrogen purification materials and high hydrogen storage medium with further lithium doping. <i>International Journal of Hydrogen Energy</i> , <b>2013</b> , 38, 9811-9818	6.7	33
109	Single-ion anisotropy, Dzyaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-12 pyrochlore R <sub>2</sub> V <sub>2</sub> O <sub>7</sub> . <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	33
108	Superhalogens as building blocks of two-dimensional organic-inorganic hybrid perovskites for optoelectronics applications. <i>Nanoscale</i> , <b>2016</b> , 8, 17836-17842	7.7	32
107	Efficient Carrier Separation and Band Structure Tuning of Two-Dimensional C <sub>2</sub> N/GaTe van der Waals Heterostructure. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 15892-15902	3.8	32
106	Electride: from computational characterization to theoretical design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2016</b> , 6, 430-440	7.9	31
105	Electronic structure of atomic Ti chains on semiconducting graphene nanoribbons: a first-principles study. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 164706	3.9	30

104	Progress and prospects in low-dimensional multiferroic materials. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2019</b> , 9, e1409	7.9	30
103	Accurate K-edge X-ray photoelectron and absorption spectra of g-CN nanosheets by first-principles simulations and reinterpretations. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 22819-22830	3.6	29
102	Theoretical understanding of magnetic and electronic structures of Ti3C2 monolayer and its derivatives. <i>Solid State Communications</i> , <b>2015</b> , 222, 9-13	1.6	28
101	Electronic properties and hydrogen storage application of designed porous nanotubes from a polyphenylene network. <i>International Journal of Hydrogen Energy</i> , <b>2014</b> , 39, 18966-18975	6.7	28
100	Theoretical analysis of the spin exchange and magnetic dipole-dipole interactions leading to the magnetic structure of Ni3TeO6. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 7545-8	5.1	28
99	Origin of the Ising ferrimagnetism and spin-charge coupling in LuFe2O4. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	27
98	High-temperature ferro-electricity in two-dimensional atomic crystal. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 193103	3.4	26
97	Water-sprouted, plasma-enhanced Ni-Co phospho-nitride nanosheets boost electrocatalytic hydrogen and oxygen evolution. <i>Chemical Engineering Journal</i> , <b>2020</b> , 402, 126257	14.7	26
96	Quantum Phase Transition in Germanene and Stanene Bilayer: From Normal Metal to Topological Insulator. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 1919-24	6.4	26
95	Density-functional analysis of spin exchange and ferroelectric polarization in AgCrO2. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	25
94	Theoretical Investigation of the Magnetic Structure and Ferroelectric Polarization of the Multiferroic Langasite Ba3NbFe3Si2O14. <i>Chemistry of Materials</i> , <b>2010</b> , 22, 5290-5295	9.6	24
93	Orbital order and partial electronic delocalization in a triangular magnetic metal Ag2MnO2. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	23
92	Prediction of another semimetallic silicene allotrope with Dirac fermions. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2017</b> , 381, 3754-3759	2.3	22
91	A promising two-dimensional channel material: monolayer antimonide phosphorus. <i>Science China Materials</i> , <b>2016</b> , 59, 648-656	7.1	22
90	Two-dimensional organometallic porous sheets with possible high-temperature ferromagnetism. <i>Nanoscale</i> , <b>2012</b> , 4, 5304-7	7.7	22
89	Ferroelectricity in perovskites with s0 A-site cations: toward near-room-temperature multiferroics. <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 1603-6	16.4	22
88	Mechanical, Electronic, and Magnetic Properties of NiX (X = Cl, Br, I) Layers. <i>ACS Omega</i> , <b>2019</b> , 4, 5714-5721	3.9	20
87	Ultra-High-Temperature Ferromagnetism in Intrinsic Tetrahedral Semiconductors. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 12413-12418	16.4	20

86	The effect of oxygen vacancy on the half-metallic nature of double perovskite Sr <sub>2</sub> FeMoO <sub>6</sub> : A theoretical study. <i>Solid State Communications</i> , <b>2014</b> , 177, 57-60	1.6	20
85	Tunable band gap and hydrogen adsorption property of a two-dimensional porous polymer by nitrogen substitution. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 666-70	3.6	20
84	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. <i>Npj 2D Materials and Applications</i> , <b>2019</b> , 3,	8.8	19
83	First-Principles Prediction of Room-Temperature Ferromagnetic Semiconductor MnS <sub>2</sub> via Isovalent Alloying. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 10114-10119	3.8	19
82	Density functional theory analysis of the interplay between Jahn-Teller instability, uniaxial magnetism, spin arrangement, metal-metal interaction, and spin-orbit coupling in Ca <sub>3</sub> CoMO <sub>6</sub> (M = Co, Rh, Ir). <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 1758-66	5.1	19
81	Enhancing magnetic vacancies in semiconductors by strain. <i>Applied Physics Letters</i> , <b>2012</b> , 100, 072401	3.4	19
80	Graphene Nanoribbons: Geometric, Electronic, and Magnetic Properties <b>2011</b> ,		18
79	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. <i>Solid State Communications</i> , <b>2011</b> , 151, 1228-1230	1.6	18
78	First-principles study of interaction between H <sub>2</sub> molecules and BN nanotubes with BN divacancies. <i>Journal of Chemical Physics</i> , <b>2007</b> , 127, 164718	3.9	18
77	Discovery of twin orbital-order phases in ferromagnetic semiconducting VI monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 512-517	3.6	18
76	Pi-back-donation effect of the cyanide ligands on the electron correlation and charge transfer in Prussian blue RbMn[Fe(CN) <sub>6</sub> ]. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 3086-8	5.1	17
75	The strain effect on colossal oxygen ionic conductivity in nanoscale zirconia electrolytes: a first-principles-based study. <i>Physical Chemistry Chemical Physics</i> , <b>2013</b> , 15, 2692-7	3.6	16
74	The effect of biaxial mechanical strain on the physical properties of double perovskite Sr <sub>2</sub> FeMoO <sub>6</sub> : A theoretical study. <i>Solid State Communications</i> , <b>2014</b> , 191, 70-75	1.6	16
73	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. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 6890-7	5.1	16
72	Unzipping carbon nanotubes into nanoribbons upon oxidation: a first-principles study. <i>Nanoscale</i> , <b>2012</b> , 4, 1254-7	7.7	16
71	Geometric and Electronic Structures as well as Thermodynamic Stability of Hexyl-Modified Silicon Nanosheet. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 13283-13288	3.8	15
70	Designing half-metallic ferromagnetism by a new strategy: an example of superhalogen modified graphitic C <sub>3</sub> N <sub>4</sub> . <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 1709-1714	7.1	14
69	Biaxial strain effect on the electronic and magnetic phase transitions in double perovskite La <sub>2</sub> FeMnO <sub>6</sub> : A first-principles study. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 063713	2.5	14

68	Band gap engineering and visible light response for GaS monolayer by isovalent anion-cation codoping. <i>Materials Chemistry and Physics</i> , <b>2017</b> , 198, 275-282	4.4	13
67	Will a graphitic-like ZnO single-layer be an ideal substrate for graphene?. <i>RSC Advances</i> , <b>2014</b> , 4, 17478	3.7	13
66	The layered ferromagnet Cs <sub>2</sub> AgF <sub>4</sub> : Antiferromagnetic inter-layer coupling driven by magnetic dipole-dipole interactions. <i>Zeitschrift für Kristallographie</i> , <b>2010</b> , 225,		13
65	First-principles calculations of the electronic and magnetic properties of Cs <sub>2</sub> AgF <sub>4</sub> . <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	13
64	Prediction of room-temperature ferromagnetism in a two-dimensional direct band gap semiconductor. <i>Nanoscale</i> , <b>2020</b> , 12, 15670-15676	7.7	12
63	High-capacity hydrogen storage in Li-adsorbed g-C <sub>3</sub> N <sub>4</sub> . <i>Materials Chemistry and Physics</i> , <b>2016</b> , 180, 440-444	4.4	12
62	Edge-Modified Graphene Nanoribbons: Appearance of Robust Spiral Magnetism. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 1371-1376	3.8	11
61	A B-C-N hybrid porous sheet: an efficient metal-free visible-light absorption material. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 4299-304	3.6	11
60	Electrical rectification by selective wave-function coupling in small Ag clusters on Si(111)( $\sqrt{7}\times\sqrt{7}$ ). <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	11
59	On the importance of the interplaquette spin exchanges in Na <sub>3</sub> RuO <sub>4</sub> : density functional theory analysis of the spin exchange and magnetic properties. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 3025-8	5.1	11
58	Influences of lithium doping and fullerene impregnation on hydrogen storage in metal organic frameworks. <i>Molecular Simulation</i> , <b>2013</b> , 39, 968-974	2	10
57	Analysis of the magnetic structure and ferroelectric polarization of monoclinic MnSb(2)S(4) by density functional theory calculations. <i>Inorganic Chemistry</i> , <b>2010</b> , 49, 10956-9	5.1	10
56	On the high magnetic-ordering temperature of the 5d magnetic oxide Ca <sub>3</sub> LiOsO <sub>6</sub> crystallizing in a trigonal crystal structure: density functional analysis. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 4182-6	5.1	10
55	Tuning Electronic and Magnetic Properties of Two-Dimensional Ferromagnetic Semiconductor CrI <sub>3</sub> through Adsorption of Benzene. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 22143-22149	3.8	10
54	A promising way to open an energy gap in bilayer graphene. <i>Nanoscale</i> , <b>2015</b> , 7, 17096-101	7.7	9
53	Boosting the high-capacity with multi-active centers: A first-principles investigation of NiPS <sub>3</sub> monolayer as an anode material. <i>Applied Surface Science</i> , <b>2019</b> , 495, 143534	6.7	9
52	Stability of graphitic-like zinc oxide layers under carriers doping: a first-principles study. <i>Nanoscale</i> , <b>2013</b> , 5, 12111-4	7.7	9
51	Two-dimensional silicon monolayers generated on c-BN(111) substrate. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 15694-700	3.6	9

50	d0 magnetism in semiconductors through confining delocalized atomic orbitals. <i>Applied Physics Letters</i> , <b>2013</b> , 102, 022422	3.4	9
49	Half-metallicity obtained in silicene nanosheet by nitrogenation engineering. <i>Journal of Applied Physics</i> , <b>2016</b> , 120, 234303	2.5	9
48	Computational Dissection of 2D SiC7 Monolayer: A Direct Band Gap Semiconductor and High Power Conversion Efficiency. <i>Advanced Theory and Simulations</i> , <b>2019</b> , 2, 1900058	3.5	8
47	Ferroelectricity in Perovskites with s0 A-Site Cations: Toward Near-Room-Temperature Multiferroics. <i>Angewandte Chemie</i> , <b>2010</b> , 122, 1647-1650	3.6	8
46	Vacancy-induced insulator $\rightarrow$ direct spin gapless semiconductor $\rightarrow$ half-metal transition in double perovskite La <sub>2</sub> CrFeO <sub>6</sub> : A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2015</b> , 379, 2897-2901	2.3	7
45	Carrier-tunable magnetism of graphene with single-atom vacancy. <i>Journal of Applied Physics</i> , <b>2013</b> , 113, 213709	2.5	7
44	Tunable ferroelectric single-atom catalysis of CO oxidation using a Pt/In <sub>2</sub> Se <sub>3</sub> monolayer. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 20725-20731	13	7
43	Trimetallic Octahedral Ni <sub>100</sub> W Phosphoxide Sprouted from Plasma-Defect-Engineered Ni <sub>100</sub> Support for Ultrahigh-Performance Electrocatalytic Hydrogen Evolution. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2021</b> , 9, 7454-7465	8.3	7
42	Quinone-Facilitated Coordinated Bipyrene and Polypyrene on Au(111) by Capture of Gold Adatoms. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 16281-16287	3.8	6
41	Ferroelectric-like structural transition in metallic LiOsO <sub>3</sub> . <i>RSC Advances</i> , <b>2014</b> , 4, 26843	3.7	6
40	Density Functional Investigation of the Difference in the Magnetic Structures of the Layered Triangular Antiferromagnets CuFeO <sub>2</sub> and AgCrO <sub>2</sub> . <i>Chemistry of Materials</i> , <b>2011</b> , 23, 4181-4185	9.6	6
39	Room-Temperature Ferroelectricity in 1T <sup>-1</sup> ReS <sub>2</sub> Multilayers. <i>Physical Review Letters</i> , <b>2022</b> , 128, 067601	7.4	5
38	Controllable vdW Contacts between the Ferroelectric In <sub>2</sub> Se <sub>3</sub> Monolayer and Two-Dimensional Metals. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 10738-10746	3.8	5
37	Valley contrasting in epitaxial growth of In/Tl homoatomic monolayer with anomalous Nernst conductance. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	5
36	Atomically dispersed tungsten on metal halide monolayer as a ferromagnetic Chern insulator. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	5
35	Effect of Coulomb Correlation on the Magnetic Properties of Mn Clusters. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 4350-4356	2.8	4
34	Theoretical study of CO oxidation on cationic, neutral, and anionic AuM dimers (M = Pd and Ag). <i>Journal of Molecular Modeling</i> , <b>2014</b> , 20, 2313	2	4
33	First-principles investigations on the magnetic structure of $\beta$ -NaMnO <sub>3</sub> <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 456002	1.8	4



32	Built-in electric field control of magnetic coupling in van der Waals semiconductors. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	4
31	Hexagonal Boron Nitride/Metal Junction: Removing the Schottky Barriers by Grain Boundary. <i>Advanced Theory and Simulations</i> , <b>2018</b> , 1, 1800045	3.5	4
30	Realizing half-metallicity in K <sub>2</sub> CoF <sub>4</sub> exfoliated nanosheets via defect engineering. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 15765-73	3.6	3
29	Magnetic structure of (C <sub>5</sub> H <sub>12</sub> N)CuBr <sub>3</sub> : origin of the uniform Heisenberg chain behavior and the magnetic anisotropy of the Cu <sup>2+</sup> (S = 1/2) ions. <i>RSC Advances</i> , <b>2016</b> , 6, 22722-22727	3.7	3
28	Atomically thin mononitrides SiN and GeN: New two-dimensional wide band gap semiconductors. <i>Europhysics Letters</i> , <b>2018</b> , 122, 47002	1.6	3
27	Giant Band Gap Reduction and Insulator/Metal Transition in Two-Dimensional InX (X = Cl, Br, I) Layers. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 21763-21767	3.8	3
26	Coexistence of metallic and insulating-like states in graphene. <i>Scientific Reports</i> , <b>2015</b> , 5, 8974	4.9	3
25	Site-selected doping in silicon nanowires by an external electric field. <i>Nanoscale</i> , <b>2011</b> , 3, 3620-2	7.7	3
24	Theoretical realization of half-metallicity in two-dimensional monolayered molybdenum dinitride by Mo vacancy tuning. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2016</b> , 380, 2669-2673	2.3	3
23	Selective Construction of Magic Hierarchical Metal/Organic Clusters on Surfaces. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 358-365	3.8	3
22	Enabling High Loading in Single-Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites.. <i>Small</i> , <b>2022</b> , e2200073	11	3
21	A theoretical study on the structural and physical properties of the ground-state CaC. <i>Solid State Communications</i> , <b>2015</b> , 203, 10-15	1.6	2
20	Hydrogen Induced Etching Features of Wrinkled Graphene Domains. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	2
19	Xiang et al. reply. <i>Physical Review Letters</i> , <b>2014</b> , 112, 199802	7.4	2
18	Magnetism of semiconductor-based magnetic tunnel junctions under electric field from first principles. <i>Applied Physics Letters</i> , <b>2009</b> , 94, 252102	3.4	2
17	High-Temperature p-Orbital Half-Metallicity and Out-of-Plane Piezoelectricity in a GaN Monolayer Induced by Superhalogens. <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 10027-10033	3.8	2
16	Nature of spin-lattice coupling in two-dimensional CrI <sub>3</sub> and CrGeTe <sub>3</sub> . <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2021</b> , 64, 1	3.6	2
15	Graphene-mediated ferromagnetic coupling in the nickel nano-islands/graphene hybrid. <i>Science Advances</i> , <b>2021</b> , 7,	14.3	2

14	Two-dimensional metal-free boron chalcogenides BX (X = Se and Te) as photocatalysts for water splitting under visible light. <i>Nanoscale</i> , <b>2021</b> , 13, 3627-3632	7.7	2
13	Synthesis of Amorphous Carbon Film in Ethanol Inverse Diffusion Flames. <i>Nanomaterials</i> , <b>2018</b> , 8,	5.4	1
12	Substrate-induced half-metallic property in epitaxial silicene. <i>Europhysics Letters</i> , <b>2019</b> , 126, 57006	1.6	1
11	Band structure tuning and charge separation of MNX monolayers and MNX/GaS van der Waals heterostructures. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2019</b> , 108, 44-52	3	1
10	Dimension effect on ferroelectricity: a first-principles study on GeS nanoribbons. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 18863-18868	3.6	1
9	Unconventional distortion induced two-dimensional multiferroicity in a CrO monolayer. <i>Nanoscale</i> , <b>2021</b> , 13, 13048-13056	7.7	1
8	Giant Biquadratic Exchange in 2D Magnets and Its Role in Stabilizing Ferromagnetism of NiCl <sub>2</sub> Monolayers.. <i>Physical Review Letters</i> , <b>2021</b> , 127, 247204	7.4	1
7	Enabling High Loading in Single-Atom Catalysts on Bare Substrate with Chemical Scissors by Saturating the Anchoring Sites (Small 19/2022). <i>Small</i> , <b>2022</b> , 18, 2270098	11	1
6	Manipulating the Raman scattering rotation magnetic field in an MoS monolayer.. <i>RSC Advances</i> , <b>2021</b> , 11, 4035-4041	3.7	0
5	Magnetic and electronic properties of frustrated spin dimer compound K <sub>2</sub> Fe <sub>2</sub> B <sub>2</sub> O <sub>7</sub> : A first-principles calculation. <i>Solid State Communications</i> , <b>2015</b> , 220, 77-80	1.6	
4	Surface-sensitive magnetic characterization technique for ultrathin ferromagnetic film with perpendicular magnetic anisotropy. <i>AIP Advances</i> , <b>2020</b> , 10, 065019	1.5	
3	Modulation on the Iron Centers by Selective Synthesis of Organic Ligands with Stereo-Specific Conformations. <i>Small</i> , <b>2021</b> , 17, e2008036	11	
2	Transition between half-metal and ferromagnetic semiconductor induced by silicon vacancy in bulk non-metallic substrate supported silicene. <i>Journal Physics D: Applied Physics</i> , <b>2021</b> , 54, 125302	3	
1	Improved contact properties of graphene-metal hybrid interfaces by grain boundaries. <i>Applied Surface Science</i> , <b>2021</b> , 563, 150392	6.7	