

# Rajeev Ahuja

## List of Publications by Year in descending order

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g-index

987  
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987  
docs citations

987  
times ranked

30322  
citing authors

#	ARTICLE	IF	CITATIONS
1	Dimensionality effects in high-performance thermoelectric materials: Computational and experimental progress in energy harvesting applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1547.	14.6	20
2	Exploring the relationship between Ln leaching and Ln-O binding energy in monazite (Nd, Sm, Eu). Journal of the American Ceramic Society, 2022, 105, 553-563.	3.8	5
3	Two-dimensional Nitrogenated Holey Graphene (C <sub>2</sub> N) monolayer based glucose sensor for diabetes mellitus. Applied Surface Science, 2022, 573, 151579.	6.1	20
4	Asymmetry-Induced Redistribution in Sn(IV)-Ti(IV) Hetero-Bimetallic Alkoxide Precursors and Its Impact on Thin-Film Deposition by Metal-Organic Chemical Vapor Deposition. Crystal Growth and Design, 2022, 22, 54-59.	3.0	1
5	Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis. Green Chemistry, 2022, 24, 1190-1210.	9.0	23
6	First-principles calculations to investigate electronic structure and optical properties of 2D MgCl <sub>2</sub> monolayer. Superlattices and Microstructures, 2022, 162, 107132.	3.1	15
7	Thermophysical properties of helium and hydrogen mixtures under high pressure predicted by ab-initio calculations: Implications for Saturn and Jupiter planets. Chemical Physics, 2022, 555, 111430.	1.9	0
8	Roles of optical phonons and logarithmic profile of electron-phonon coupling integration in superconducting Sc <sub>0.5</sub> Y <sub>0.5</sub> Hf <sub>6</sub> superhydride under pressures. Journal of Alloys and Compounds, 2022, 901, 163524.	5.5	11
9	Binding and optical characteristics of polycyclic aromatic hydrocarbons and their nitroderivatives adsorbed on the C <sub>3</sub> N monolayer. New Journal of Chemistry, 2022, 46, 2245-2258.	2.8	7
10	Elucidating the reaction pathway of crystalline multi-metal borides for highly efficient oxygen-evolving electrocatalysts. Journal of Materials Chemistry A, 2022, 10, 1569-1578.	10.3	13
11	Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solid-liquid interfaces. Nanoscale Advances, 2022, 4, 884-893.	4.6	4
12	Two-Dimensional Perovskite/HfS <sub>2</sub> van der Waals Heterostructure as an Absorber Material for Photovoltaic Applications. ACS Applied Energy Materials, 2022, 5, 2300-2307.	5.1	9
13	Modified KBBF-like Material for Energy Storage Applications: ZnNiBO <sub>3</sub> (OH) with Enhanced Cycle Life. ACS Applied Materials & Interfaces, 2022, 14, 8025-8035.	8.0	20
14	Pressure induced structural phase transition and piezochromism in photovoltaic sillen compounds PbBiO <sub>2</sub> X (X=Cl, Br & I). Applied Materials Today, 2022, 26, 101372.	4.3	0
15	Exotic magnetic and electronic properties of layered CrI <sub>3</sub> single crystals under high pressure. Physical Review B, 2022, 105, .	3.2	12
16	Strain-mediated ferromagnetism and low-field magnetic reversal in Co doped monolayer WS <sub>2</sub> . Scientific Reports, 2022, 12, 2593.	3.3	10
17	Relativistic Effects in Platinum Nanocluster Catalysis: A Statistical Ensemble-Based Analysis. Journal of Physical Chemistry A, 2022, 126, 1345-1359.	2.5	7
18	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. ACS Applied Nano Materials, 2022, 5, 2984-2993.	5.0	29

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19	Strain modulating electronic band gaps and SQ efficiencies of semiconductor 2D PdQ <sub>2</sub> (Q = S, Se) monolayer. <i>Scientific Reports</i> , 2022, 12, 2964.	3.3	19
20	Zn-Co-MOF on solution-free CuO nanowires for flexible hybrid energy storage devices. <i>Materials Today Physics</i> , 2022, 23, 100655.	6.0	35
21	Electronic bandstructure modulation of MoX <sub>2</sub> /ZnO(X:S,Se) heterostructure by applying external electric field. <i>Surfaces and Interfaces</i> , 2022, 29, 101817.	3.0	8
22	Progress and challenges in layered two-dimensional hybrid perovskites. <i>Nanotechnology</i> , 2022, 33, 292501.	2.6	11
23	Revealing the superlative electrochemical properties of o-B <sub>2</sub> N <sub>2</sub> monolayer in Lithium/Sodium-ion batteries. <i>Nano Energy</i> , 2022, 96, 107066.	16.0	29
24	2D Janus and non-Janus diamanes with an in-plane negative Poisson's ratio for energy applications. <i>Materials Today Advances</i> , 2022, 14, 100225.	5.2	10
25	Janus Aluminum Oxysulfide Al <sub>2</sub> OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. <i>Applied Surface Science</i> , 2022, 589, 152997.	6.1	21
26	Structures, stabilities, optoelectronic and photocatalytic properties of Janus aluminium mono-chalcogenides Al(Ga, In)STe monolayers. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2022, 142, 115229.	2.7	2
27	Stabilizing superconductivity of ternary metal pentahydride $\text{CaCH}_5$ via electronic topological transitions under high pressure from first principles evolutionary algorithm. <i>Scientific Reports</i> , 2022, 12, 6700.	3.3	3
28	TM dopant-induced H-vacancy diffusion kinetics of sodium-lithium alanates: Ab initio study for hydrogen storage improvement. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 18763-18771.	7.1	11
29	Activation-induced Surface Modulation of Biowaste-derived Hierarchical Porous Carbon for Supercapacitors. <i>ChemPlusChem</i> , 2022, 87, .	2.8	18
30	Bifunctional catalytic activity of 2D boron monochalcogenides BX (X = S, Se, Te). <i>Materials Today Energy</i> , 2022, 27, 101026.	4.7	7
31	Flexible 3D porous boron nitride interconnected network as a high-performance Li-and Na-ion battery electrodes. <i>Electrochimica Acta</i> , 2022, 421, 140491.	5.2	9
32	Probing the electronic, optical and transport properties of halide double perovskites Rb <sub>2</sub> InSb(Cl,Br) <sub>6</sub> for solar cells and thermoelectric applications. <i>Journal of Solid State Chemistry</i> , 2022, 312, 123262.	2.9	10
33	Prominent Electrode Material for Na-, K-, and Mg-ion Batteries: 2D $\hat{I}^2$ -Sb Monolayer. <i>Energy &amp; Fuels</i> , 2022, 36, 7087-7095.	5.1	16
34	Tuning the electronic, magnetic, and sensing properties of a single atom embedded microporous C <sub>3</sub> N <sub>6</sub> monolayer towards XO <sub>2</sub> (X = C, N, S) gases. <i>New Journal of Chemistry</i> , 2022, 46, 13752-13765.	2.8	5
35	Optoelectronic properties of 2D van der Waals heterostructure As/PtS <sub>2</sub> by first-principles calculations. <i>Materials Today: Proceedings</i> , 2022, 67, 250-253.	1.8	1
36	Transition metal substituted MoS <sub>2</sub> /WS <sub>2</sub> van der Waals heterostructure for realization of dilute magnetic semiconductors. <i>Journal of Magnetism and Magnetic Materials</i> , 2022, 560, 169567.	2.3	6

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37	Impact of stacking on the optoelectronic properties of 2D ZrS <sub>2</sub> /GaS heterostructure. Materials Today: Proceedings, 2021, 47, 526-528.	1.8	9
38	Novel green phosphorene as a superior chemical gas sensing material. Journal of Hazardous Materials, 2021, 401, 123340.	12.4	71
39	Exploring Janus MoSSe monolayer as a workable media for SOF <sub>6</sub> decompositions sensing based on DFT calculations. Computational Materials Science, 2021, 186, 109976.	3.0	21
40	Modulation of 2D GaS/BTe vdW heterostructure as an efficient HER catalyst under external electric field influence. Catalysis Today, 2021, 370, 14-25.	4.4	20
41	Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX <sub>2</sub> monolayer. Journal of Materials Science, 2021, 56, 3846-3860.	3.7	24
42	Bain Deformation Mechanism and Lifshitz Transition in Magnesium under High Pressure. Physica Status Solidi (B): Basic Research, 2021, 258, 2000279.	1.5	8
43	Mechanism of formaldehyde and formic acid formation on (101)-TiO <sub>2</sub> @Cu <sub>4</sub> systems through CO <sub>2</sub> hydrogenation. Sustainable Energy and Fuels, 2021, 5, 564-574.	4.9	4
44	Structural, electronic and optical properties of two-dimensional Janus transition metal oxides MXO (M=Ti, Hf and Zr; X=S and Se) for photovoltaic and opto-electronic applications. Physica B: Condensed Matter, 2021, 604, 412621.	2.7	24
45	Thermodynamics and kinetics of 2D g-GeC monolayer as an anode materials for Li/Na-ion batteries. Journal of Power Sources, 2021, 485, 229318.	7.8	60
46	Selective decoration of nitrogenated holey graphene (C <sub>2</sub> N) with titanium clusters for enhanced hydrogen storage application. International Journal of Hydrogen Energy, 2021, 46, 7371-7380.	7.1	63
47	Cs <sub>2</sub> InGaX <sub>6</sub> (X=Cl, Br, or I): Emergent Inorganic Halide Double Perovskites with enhanced optoelectronic characteristics. Current Applied Physics, 2021, 21, 50-57.	2.4	48
48	Integration of CuO nanosheets to Zn-Ni-Co oxide nanowire arrays for energy storage applications. Chemical Engineering Journal, 2021, 413, 127570.	12.7	70
49	Scavenging properties of yttrium nitride monolayer towards toxic sulfur gases. Applied Surface Science, 2021, 537, 147711.	6.1	8
50	Van der Waals Heterostructure-Based Anode Materials. , 2021, , 1-18.		0
51	No-Carbon 2D Anode Materials for Next-Generation Batteries. , 2021, , 1-14.		0
52	Introduction: Background of Computational and Experimental Investigations for Next-Generation Efficient Battery Materials. , 2021, , 1-34.		0
53	An oriented Ni-Co-MOF anchored on solution-free 1D CuO: a n heterojunction for supercapacitive energy storage. Journal of Materials Chemistry A, 2021, 9, 17790-17800.	10.3	86
54	Hydrogenation and oxidation enhances the thermoelectric performance of Si <sub>2</sub> BN monolayer. New Journal of Chemistry, 2021, 45, 3892-3900.	2.8	8

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55	Pressure-promoted highly-ordered Fe-doped-Ni <sub>2</sub> S <sub>3</sub> for effective oxygen evolution reaction and overall water splitting. Journal of Materials Chemistry A, 2021, 9, 6469-6475.	10.3	37
56	Data-Driven Machine Learning Approaches for Advanced Battery Modeling. , 2021, , 1-18.		0
57	Determining factors for the nano-biocompatibility of cobalt oxide nanoparticles: proximal discrepancy in intrinsic atomic interactions at differential vicinane. Green Chemistry, 2021, 23, 3439-3458.	9.0	38
58	Formation of Lightweight Ternary Polyhydrides and Their Hydrogen Storage Mechanism. Journal of Physical Chemistry C, 2021, 125, 1723-1730.	3.1	19
59	Suitable Electrode Materials for Hybrid Capacitors. , 2021, , 1-30.		0
60	MXene-Based 2D Anode Materials for Next-Generation Batteries. , 2021, , 1-20.		1
61	Graphene-Based Anode Materials for Li and Na Batteries. , 2021, , 1-24.		0
62	Design of Continuous Transport of the Droplet by the Contact-Boiling Regime. Langmuir, 2021, 37, 553-560.	3.5	8
63	Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO <sub>2</sub> Resistive Random Access Memory Device. Journal of Physical Chemistry Letters, 2021, 12, 1876-1884.	4.6	20
64	8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index. Physical Review B, 2021, 103, .	3.2	26
65	Stabilization and electronic topological transition of hydrogen-rich metal Li <sub>5</sub> MoH <sub>11</sub> under high pressures from first-principles predictions. Scientific Reports, 2021, 11, 4079.	3.3	12
66	Large-Scale Fabrication of Wettability-Controllable Coatings for Optimizing Condensate Transfer Ability. Langmuir, 2021, 37, 2476-2484.	3.5	4
67	Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nanopepper. Nanomedicine, 2021, 16, 307-322.	3.3	9
68	Large-Scale Screening of Interface Parameters in the WC/W System Using Classical Force Field and First-Principles Calculations. Journal of Physical Chemistry C, 2021, 125, 3631-3639.	3.1	3
69	Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. ACS Applied Electronic Materials, 2021, 3, 733-742.	4.3	13
70	From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. Energy & Fuels, 2021, 35, 6282-6288.	5.1	10
71	Enthalpy stabilization of superconductivity in an alloying S-P-H system: First-principles cluster expansion study under high pressure. Computational Materials Science, 2021, 190, 110282.	3.0	20
72	Salt-assisted growth of monolayer MoS <sub>2</sub> for high-performance hysteresis-free field-effect transistor. Journal of Applied Physics, 2021, 129, .	2.5	19

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73	Carbon Nitride Monolayers as Efficient Immobilizers toward Lithium Selenides: Potential Applications in Lithium–Selenium Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 3891-3904.	5.1	10
74	Antimonene Allotropes $\hat{1}$ - and $\hat{2}$ -Phases as Promising Anchoring Materials for Lithium–Sulfur Batteries. <i>Energy &amp; Fuels</i> , 2021, 35, 9001-9009.	5.1	15
75	Density Functional Theory Study on Sensing and Dielectric Properties of Arsenic Trisulfide Nanosheets for Detecting Volatile Organic Compounds. <i>ACS Applied Nano Materials</i> , 2021, 4, 5444-5453.	5.0	9
76	Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 20586-20593.	7.1	17
77	Substituted 2D Janus WSSe monolayers as efficient nanosensor toward toxic gases. <i>Journal of Applied Physics</i> , 2021, 130, .	2.5	16
78	Understanding carbon dioxide capture on metal–organic frameworks from first-principles theory: The case of MIL-53(X), with X = Fe <sup>3+</sup> , Al <sup>3+</sup> , and Cu <sup>2+</sup> . <i>Journal of Chemical Physics</i> , 2021, 155, 024701.	3.0	6
79	Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. <i>Journal of Computational Chemistry</i> , 2021, 42, 1944-1958.	3.3	4
80	Exploring the Full Potential of Functional Si <sub>2</sub> BN Nanoribbons As Highly Reversible Anode Materials for Mg-Ion Battery. <i>Energy &amp; Fuels</i> , 2021, 35, 12688-12699.	5.1	3
81	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. <i>Applied Surface Science</i> , 2021, 556, 149561.	6.1	31
82	High-Specific-Capacity and High-Performing Post-Lithium-Ion Battery Anode over 2D Black Arsenic Phosphorus. <i>ACS Applied Energy Materials</i> , 2021, 4, 7900-7910.	5.1	19
83	Application of germanene monolayers as efficient anchoring material to immobilize lithium polysulfides in Li-S batteries. <i>Applied Surface Science</i> , 2021, 558, 149850.	6.1	8
84	High-temperature superconductor of sodalite-like clathrate hafnium hexahydride. <i>Scientific Reports</i> , 2021, 11, 16403.	3.3	9
85	Empowering hydrogen storage properties of haeckelite monolayers via metal atom functionalization. <i>Applied Surface Science</i> , 2021, 556, 149709.	6.1	20
86	Nitrogen-Containing Gas Sensing Properties of 2-D Ti <sub>2</sub> N and Its Derivative Nanosheets: Electronic Structures Insight. <i>Nanomaterials</i> , 2021, 11, 2459.	4.1	5
87	Altered electrochemical properties of iron oxide nanoparticles by carbon enhance molecular biocompatibility through discrepant atomic interaction. <i>Materials Today Bio</i> , 2021, 12, 100131.	5.5	6
88	Electric Field-Modulated Charge Transfer in Geometrically Tailored MoX <sub>2</sub> /WX <sub>2</sub> (X = S, Se) Heterostructures. <i>Journal of Physical Chemistry C</i> , 2021, 125, 22360-22369.	3.1	15
89	Drastic reduction of thermal conductivity in hexagonal AX (A = Ga, In & Tl, X = As, Se & Te) monolayers due to alternative atomic configuration. <i>Nano Energy</i> , 2021, 88, 106248.	16.0	19
90	Electronic, optical and thermoelectric properties of two-dimensional pentagonal SiGeC <sub>4</sub> nanosheet for photovoltaic applications: First-principles calculations. <i>Superlattices and Microstructures</i> , 2021, 158, 107024.	3.1	9

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91	Two-dimensional Janus Sn <sub>2</sub> SSe and SnGeS <sub>2</sub> semiconductors as strong absorber candidates for photovoltaic solar cells: First principles computations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021, 134, 114900.	2.7	20
92	Binder-free trimetallic phosphate nanosheets as an electrode: Theoretical and experimental investigation. <i>Journal of Power Sources</i> , 2021, 513, 230556.	7.8	45
93	Enhanced overall water splitting under visible light of MoSSe/WSSe heterojunction by lateral interfacial engineering. <i>Journal of Catalysis</i> , 2021, 404, 18-31.	6.2	13
94	Dissociation of air pollutants on the uniform surface of pentagonal BeP <sub>2</sub> . <i>Applied Surface Science</i> , 2021, 570, 151061.	6.1	3
95	Organic Batteries: the Route Toward Sustainable Electrical Energy Storage Technologies. , 2021, , 1-22.		2
96	Influence of vacancy and adatom defects on the optoelectronic properties of monolayer GeS. <i>AIP Conference Proceedings</i> , 2021, , .	0.4	0
97	Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications. <i>Catalysis Science and Technology</i> , 2021, 11, 4996-5013.	4.1	18
98	Future Outlook and Direction of Next-Generation Battery Materials. , 2021, , 1-22.		0
99	Computational and Experimental Techniques to Envisage Battery Materials. , 2021, , 1-22.		0
100	MXene binder stabilizes pseudocapacitance of conducting polymers. <i>Journal of Materials Chemistry A</i> , 2021, 9, 20356-20361.	10.3	15
101	Local electrocatalytic activity of PtRu supported on nitrogen-doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy. <i>Journal of Materials Chemistry A</i> , 2021, 9, 21291-21301.	10.3	18
102	Harnessing the unique properties of MXenes for advanced rechargeable batteries. <i>JPhys Energy</i> , 2021, 3, 012005.	5.3	14
103	Pressure-induced order-disorder transitions in $\text{In}_2\text{S}_3$ : an experimental and theoretical study of structural and vibrational properties. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23625-23642.	2.8	3
104	Polypeptoid Material as an Anchoring Material for Li-S Batteries. <i>ACS Applied Energy Materials</i> , 2021, 4, 13070-13076.	5.1	8
105	Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space. <i>ACS Omega</i> , 2021, 6, 33240-33252.	3.5	9
106	Tuning the Nanoparticle Interfacial Properties and Stability of the Core-Shell Structure in Zn-Doped NiMoO <sub>4</sub> @AWO <sub>4</sub> . <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 56116-56130.	8.0	30
107	Theoretical Prediction of a Bi-Doped $\text{In}_2\text{S}_3$ -Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 56254-56264.	8.0	10
108	Fabrication of BP2T functionalized graphene via non-covalent $\pi$ - $\pi$ stacking interactions for enhanced ammonia detection. <i>RSC Advances</i> , 2021, 11, 35982-35987.	3.6	2

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109	Electronic and optical properties of ZnO nanosheet doped and codoped with Be and/or Mg for ultraviolet optoelectronic technologies: density functional calculations. <i>Physica Scripta</i> , 2020, 95, 015804.	2.5	17
110	Investigating CO <sub>2</sub> storage properties of C <sub>2</sub> N monolayer functionalized with small metal clusters. <i>Journal of CO<sub>2</sub> Utilization</i> , 2020, 35, 1-13.	6.8	20
111	Examination of the Magnetic Properties of the Triangular Type Mixed spin-(1/2, 1) Nanowire. <i>Journal of Superconductivity and Novel Magnetism</i> , 2020, 33, 817-824.	1.8	8
112	Progress in supercapacitors: roles of two dimensional nanotubular materials. <i>Nanoscale Advances</i> , 2020, 2, 70-108.	4.6	164
113	Orbital hybridization-induced band offset phenomena in Ni <sub>x</sub> Cd <sub>1-x</sub> O thin films. <i>Nanoscale</i> , 2020, 12, 669-686.	5.6	11
114	Li-decorated carbyne for hydrogen storage: charge induced polarization and van't Hoff hydrogen desorption temperature. <i>Sustainable Energy and Fuels</i> , 2020, 4, 691-699.	4.9	24
115	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C <sub>3</sub> N <sub>4</sub> ) nanosheets under selected transition metal doping. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 3035-3045.	7.1	110
116	Boron-Rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity. <i>Chemistry of Materials</i> , 2020, 32, 459-467.	6.7	35
117	Terahertz plasmonics: The rise of toroidal metadevices towards immunobiosensings. <i>Materials Today</i> , 2020, 32, 108-130.	14.2	271
118	Insights into the trapping mechanism of light metals on C <sub>2</sub> N-h <sub>2</sub> D: Utilisation as an anode material for metal ion batteries. <i>Carbon</i> , 2020, 160, 125-132.	10.3	29
119	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. <i>Catalysts</i> , 2020, 10, 1111.	3.5	35
120	Improved Adsorption and Migration of Divalent Ions Over C <sub>4</sub> N Nanosheets: Potential Anode for Divalent Batteries. <i>Surfaces and Interfaces</i> , 2020, 21, 100758.	3.0	5
121	Superior Anchoring of Sodium Polysulfides to the Polar C <sub>2</sub> N 2D Material: A Potential Electrode Enhancer in Sodium-Sulfur Batteries. <i>Langmuir</i> , 2020, 36, 13104-13111.	3.5	27
122	Excitonic effects in the optoelectronic properties of graphene-like BC monolayer. <i>Optical Materials</i> , 2020, 110, 110476.	3.6	19
123	Exploring the Degradation Behavior of Ce-Monazite in Water Solution through Adsorption and Penetration Kinetics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22173-22184.	3.1	10
124	Tuning Hydrogen Storage Properties of Carbon Nanosheets through Selected Foreign Metal Functionalization. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16827-16837.	3.1	15
125	Bulk and monolayer As <sub>2</sub> S <sub>3</sub> as promising thermoelectric material with high conversion performance. <i>Computational Materials Science</i> , 2020, 183, 109913.	3.0	24
126	Rational Design of 2D h-BAs Monolayer as Advanced Sulfur Host for High Energy Density Li-S Batteries. <i>ACS Applied Energy Materials</i> , 2020, 3, 7306-7317.	5.1	23



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127	Core-shell nanostructures: perspectives towards drug delivery applications. Journal of Materials Chemistry B, 2020, 8, 8992-9027.	5.8	127
128	Emerging piezochromism in transparent lead free perovskite Rb <sub>3</sub> X <sub>2</sub> I <sub>9</sub> (X = Sb, Bi) under compression: A comparative theoretical insight. Journal of Applied Physics, 2020, 128, 045102.	2.5	5
129	Reaction coordinate mapping of hydrogen evolution mechanism on Mg <sub>3</sub> N <sub>2</sub> monolayer. International Journal of Hydrogen Energy, 2020, 45, 22848-22854.	7.1	7
130	Ultrathin nanowire PdX <sub>2</sub> (X = P, As): stability, electronic transport and thermoelectric properties. New Journal of Chemistry, 2020, 44, 15617-15624.	2.8	3
131	Turning indium oxide into high-performing electrode materials via cation substitution strategy: Preserving single crystalline cubic structure of 2D nanoflakes towards energy storage devices. Journal of Power Sources, 2020, 480, 228873.	7.8	53
132	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS <sub>3</sub> (A = Tl, ET, Q, O, O, rg, BT, Overlock, 10, T, F)	5.5	24
133	Route to high- $T_c$ superconductivity of $\text{hBC}_{7}$ via strong bonding of boron-carbon compound at high pressure. Scientific Reports, 2020, 10, 18090.	3.3	11
134	Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. ChemCatChem, 2020, 12, 6013-6023.	3.7	20
135	Temperature-Dependent Cationic Doping-Driven Phonon Dynamics Investigation in CdO Thin Films Using Raman Spectroscopy. Journal of Physical Chemistry C, 2020, 124, 21818-21828.	3.1	4
136	Toroidal Metaphotonics and Metadevices. Laser and Photonics Reviews, 2020, 14, 1900326.	8.7	95
137	Zn Metal Atom Doping on the Surface Plane of One-Dimensional NiMoO <sub>4</sub> Nanorods with Improved Redox Chemistry. ACS Applied Materials & Interfaces, 2020, 12, 44815-44829.	8.0	67
138	Optical excitations and thermoelectric properties of two-dimensional holey graphene. Physical Review B, 2020, 102, .	3.2	28
139	Recent progress of defect chemistry on 2D materials for advanced battery anodes. Chemistry - an Asian Journal, 2020, 15, 3390-3404.	3.3	35
140	Density Functional Theory Studies of Si <sub>2</sub> BN Nanosheets as Anode Materials for Magnesium-Ion Batteries. ACS Applied Nano Materials, 2020, 3, 9055-9063.	5.0	40
141	Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in Two-Dimensional Thallium Selenide. ACS Applied Energy Materials, 2020, 3, 9315-9325.	5.1	24
142	Elucidating hydrogen storage properties of two-dimensional siligraphene (Si <sub>8</sub> ) monolayers upon selected metal decoration. Sustainable Energy and Fuels, 2020, 4, 5578-5587.	4.9	22
143	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (X = Se) Tj ETQq1 1 0.784314 rgBT / Overlock 130	8.0	130
144	Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. Nanomaterials, 2020, 10, 2554.	4.1	17

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