

Rajeev Ahuja

List of Publications by Year in Descending Order

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

952 papers	30,026 citations	79 h-index	130 g-index
987 ext. papers	33,894 ext. citations	4.8 avg, IF	7.55 L-index

#	Paper	IF	Citations
952	Binding and optical characteristics of polycyclic aromatic hydrocarbons and their nitroderivatives adsorbed on the C ₃ N monolayer. <i>New Journal of Chemistry</i> , 2022 , 46, 2245-2258	3.6	2
951	Elucidating the reaction pathway of crystalline multi-metal borides for highly efficient oxygen-evolving electrocatalysts. <i>Journal of Materials Chemistry A</i> , 2022 , 10, 1569-1578	13	1
950	Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solid-liquid interfaces. <i>Nanoscale Advances</i> , 2022 , 4, 884-893	5.1	1
949	Modified KBBF-like Material for Energy Storage Applications: ZnNiBO(OH) with Enhanced Cycle Life.. <i>ACS Applied Materials & Interfaces</i> , 2022 ,	9.5	5
948	Pressure induced structural phase transition and piezochromism in photovoltaic sillen compounds PbBiO ₂ X (X = Cl, Br & I). <i>Applied Materials Today</i> , 2022 , 26, 101372	6.6	
947	First-principles calculations to investigate electronic structure and optical properties of 2D MgCl ₂ monolayer. <i>Superlattices and Microstructures</i> , 2022 , 162, 107132	2.8	0
946	Thermophysical properties of helium and hydrogen mixtures under high pressure predicted by ab-initio calculations: Implications for Saturn and Jupiter planets. <i>Chemical Physics</i> , 2022 , 555, 111430	2.3	
945	Roles of optical phonons and logarithmic profile of electron-phonon coupling integration in superconducting Sc _{0.5} Y _{0.5} H ₆ superhydride under pressures. <i>Journal of Alloys and Compounds</i> , 2022 , 901, 163524	5.7	2
944	Two-dimensional Nitrogenated Holey Graphene (C ₂ N) monolayer based glucose sensor for diabetes mellitus. <i>Applied Surface Science</i> , 2022 , 573, 151579	6.7	5
943	Exploring the relationship between Ln leaching and Ln-D binding energy in monazite (Nd, Sm, Eu). <i>Journal of the American Ceramic Society</i> , 2022 , 105, 553	3.8	1
942	Strain-mediated ferromagnetism and low-field magnetic reversal in Co doped monolayer [Formula: see text].. <i>Scientific Reports</i> , 2022 , 12, 2593	4.9	1
941	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. <i>ACS Applied Nano Materials</i> , 2022 , 5, 2984-2993	5.6	2
940	Strain modulating electronic band gaps and SQ efficiencies of semiconductor 2D PdQ (Q = S, Se) monolayer.. <i>Scientific Reports</i> , 2022 , 12, 2964	4.9	1
939	Zn-Co-MOF on solution-free CuO nanowires for flexible hybrid energy storage devices. <i>Materials Today Physics</i> , 2022 , 23, 100655	8	10
938	Electronic bandstructure modulation of MoX ₂ /ZnO(X:S,Se) heterostructure by applying external electric field. <i>Surfaces and Interfaces</i> , 2022 , 29, 101817	4.1	0
937	Revealing the superlative electrochemical properties of o-B ₂ N ₂ monolayer in Lithium/Sodium-ion batteries. <i>Nano Energy</i> , 2022 , 96, 107066	17.1	6
936	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	7.4	1

935	Janus Aluminum Oxysulfide Al ₂ OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. <i>Applied Surface Science</i> , 2022 , 589, 152997	6.7	3
934	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 , 115229	3	
933	Stabilizing superconductivity of ternary metal pentahydride [Formula: see text] via electronic topological transitions under high pressure from first principles evolutionary algorithm.. <i>Scientific Reports</i> , 2022 , 12, 6700	4.9	0
932	Bifunctional Catalytic Activity of 2D Boron Monochalcogenides BX (X = S, Se, Te). <i>Materials Today Energy</i> , 2022 , 101026	7	1
931	Flexible 3D porous boron nitride interconnected network as a high-performance Li-and Na-ion battery electrodes. <i>Electrochimica Acta</i> , 2022 , 421, 140491	6.7	2
930	Probing the electronic, optical and transport properties of halide double perovskites Rb ₂ InSb(Cl,Br) ₆ for solar cells and thermoelectric applications. <i>Journal of Solid State Chemistry</i> , 2022 , 123262	3.3	0
929	Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space.. <i>ACS Omega</i> , 2021 , 6, 33240-33252	3.9	0
928	Tuning the Nanoparticle Interfacial Properties and Stability of the Core-Shell Structure in Zn-Doped NiMoO@AWO. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56116-56130	9.5	4
927	Theoretical Prediction of a Bi-Doped Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56234-56244	9.5	3
926	Fabrication of BP2T functionalized graphene non-covalent π -stacking interactions for enhanced ammonia detection.. <i>RSC Advances</i> , 2021 , 11, 35982-35987	3.7	1
925	Pressure-induced order-disorder transitions in InS: an experimental and theoretical study of structural and vibrational properties. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 23625-23642	3.6	0
924	Harnessing the unique properties of MXenes for advanced rechargeable batteries. <i>JPhys Energy</i> , 2021 , 3, 012005	4.9	7
923	From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. <i>Energy & Fuels</i> , 2021 , 35, 6282-6288	4.1	2
922	Enthalpy stabilization of superconductivity in an alloying S-P-H system: First-principles cluster expansion study under high pressure. <i>Computational Materials Science</i> , 2021 , 190, 110282	3.2	10
921	Salt-assisted growth of monolayer MoS ₂ for high-performance hysteresis-free field-effect transistor. <i>Journal of Applied Physics</i> , 2021 , 129, 145106	2.5	7
920	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	6.1	5
919	Antimonene Allotropes β and β' Phases as Promising Anchoring Materials for Lithium-Sulfur Batteries. <i>Energy & Fuels</i> , 2021 , 35, 9001-9009	4.1	4
918	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	5.6	4

917	Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 20586-20593	6.7	7
916	Substituted 2D Janus WSSe monolayers as efficient nanosensor toward toxic gases. <i>Journal of Applied Physics</i> , 2021 , 130, 014501	2.5	4
915	Novel green phosphorene as a superior chemical gas sensing material. <i>Journal of Hazardous Materials</i> , 2021 , 401, 123340	12.8	32
914	Exploring Janus MoSSe monolayer as a workable media for SOF ₆ decompositions sensing based on DFT calculations. <i>Computational Materials Science</i> , 2021 , 186, 109976	3.2	11
913	Modulation of 2D GaS/BTe vdW heterostructure as an efficient HER catalyst under external electric field influence. <i>Catalysis Today</i> , 2021 , 370, 14-25	5.3	5
912	Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX ₂ monolayer. <i>Journal of Materials Science</i> , 2021 , 56, 3846-3860	4.3	8
911	Bain Deformation Mechanism and Lifshitz Transition in Magnesium under High Pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2021 , 258, 2000279	1.3	6
910	Mechanism of formaldehyde and formic acid formation on (101)-TiO ₂ @Cu ₄ systems through CO ₂ hydrogenation. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 564-574	5.8	1
909	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. <i>Physica B: Condensed Matter</i> , 2021 , 604, 412621	2.8	13
908	Thermodynamics and kinetics of 2D g-GeC monolayer as an anode materials for Li/Na-ion batteries. <i>Journal of Power Sources</i> , 2021 , 485, 229318	8.9	21
907	Selective decoration of nitrogenated holey graphene (C ₂ N) with titanium clusters for enhanced hydrogen storage application. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 7371-7380	6.7	17
906	Cs ₂ InGaX ₆ (X=Cl, Br, or I): Emergent Inorganic Halide Double Perovskites with enhanced optoelectronic characteristics. <i>Current Applied Physics</i> , 2021 , 21, 50-57	2.6	13
905	Integration of CuO nanosheets to Zn-Ni-Co oxide nanowire arrays for energy storage applications. <i>Chemical Engineering Journal</i> , 2021 , 413, 127570	14.7	24
904	Scavenging properties of yttrium nitride monolayer towards toxic sulfur gases. <i>Applied Surface Science</i> , 2021 , 537, 147711	6.7	1
903	Van der Waals Heterostructure-Based Anode Materials 2021 , 1-18		
902	No-Carbon 2D Anode Materials for Next-Generation Batteries 2021 , 1-14		
901	Introduction: Background of Computational and Experimental Investigations for Next-Generation Efficient Battery Materials 2021 , 1-34		
900	An oriented NiCo-MOF anchored on solution-free 1D CuO: a p-n heterojunction for supercapacitive energy storage. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 17790-17800	13	28

899	Hydrogenation and oxidation enhances the thermoelectric performance of Si ₂ BN monolayer. <i>New Journal of Chemistry</i> , 2021 , 45, 3892-3900	3.6	0
898	Pressure-promoted highly-ordered Fe-doped-Ni ₂ B for effective oxygen evolution reaction and overall water splitting. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 6469-6475	13	10
897	Data-Driven Machine Learning Approaches for Advanced Battery Modeling 2021 , 1-18		
896	Determining factors for the nano-biocompatibility of cobalt oxide nanoparticles: proximal discrepancy in intrinsic atomic interactions at differential vicinage. <i>Green Chemistry</i> , 2021 , 23, 3439-3458 ¹⁰		11
895	Formation of Lightweight Ternary Polyhydrides and Their Hydrogen Storage Mechanism. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 1723-1730	3.8	10
894	Suitable Electrode Materials for Hybrid Capacitors 2021 , 1-30		
893	MXene-Based 2D Anode Materials for Next-Generation Batteries 2021 , 1-20		
892	Graphene-Based Anode Materials for Li and Na Batteries 2021 , 1-24		
891	Design of Continuous Transport of the Droplet by the Contact-Boiling Regime. <i>Langmuir</i> , 2021 , 37, 553-560	5.0	2
890	Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO Resistive Random Access Memory Device. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1876-1884	6.4	7
889	8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index. <i>Physical Review B</i> , 2021 , 103,	3.3	8
888	Stabilization and electronic topological transition of hydrogen-rich metal LiMoH under high pressures from first-principles predictions. <i>Scientific Reports</i> , 2021 , 11, 4079	4.9	6
887	Large-Scale Fabrication of Wettability-Controllable Coatings for Optimizing Condensate Transfer Ability. <i>Langmuir</i> , 2021 , 37, 2476-2484	4	2
886	Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nanopepper. <i>Nanomedicine</i> , 2021 , 16, 307-322	5.6	5
885	Large-Scale Screening of Interface Parameters in the WC/W System Using Classical Force Field and First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 3631-3639	3.8	1
884	Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. <i>ACS Applied Electronic Materials</i> , 2021 , 3, 733-742	4	5
883	Understanding carbon dioxide capture on metal-organic frameworks from first-principles theory: The case of MIL-53(X), with X = Fe, Al, and Cu. <i>Journal of Chemical Physics</i> , 2021 , 155, 024701	3.9	1
882	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	3.5	1

881	Exploring the Full Potential of Functional Si ₂ BN Nanoribbons As Highly Reversible Anode Materials for Mg-Ion Battery. <i>Energy & Fuels</i> , 2021 , 35, 12688-12699	4.1	1
880	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. <i>Applied Surface Science</i> , 2021 , 556, 149561	6.7	10
879	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	6.1	1
878	Application of germanene monolayers as efficient anchoring material to immobilize lithium polysulfides in Li-S batteries. <i>Applied Surface Science</i> , 2021 , 558, 149850	6.7	4
877	High-temperature superconductor of sodalite-like clathrate hafnium hexahydride. <i>Scientific Reports</i> , 2021 , 11, 16403	4.9	2
876	Empowering hydrogen storage properties of haeckelite monolayers via metal atom functionalization. <i>Applied Surface Science</i> , 2021 , 556, 149709	6.7	4
875	Altered electrochemical properties of iron oxide nanoparticles by carbon enhance molecular biocompatibility through discrepant atomic interaction. <i>Materials Today Bio</i> , 2021 , 12, 100131	9.9	2
874	Drastic reduction of thermal conductivity in hexagonal AX (A = Ga, In & Tl, X = S, Se & Te) monolayers due to alternative atomic configuration. <i>Nano Energy</i> , 2021 , 88, 106248	17.1	3
873	Electronic, optical and thermoelectric properties of two-dimensional pentagonal SiGeC ₄ nanosheet for photovoltaic applications: First-principles calculations. <i>Superlattices and Microstructures</i> , 2021 , 158, 107024	2.8	3
872	Two-dimensional Janus Sn ₂ SSe and SnGeS ₂ semiconductors as strong absorber candidates for photovoltaic solar cells: First principles computations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 134, 114900	3	7
871	Binder-free trimetallic phosphate nanosheets as an electrode: Theoretical and experimental investigation. <i>Journal of Power Sources</i> , 2021 , 513, 230556	8.9	18
870	Enhanced overall water splitting under visible light of MoSSe WSSe heterojunction by lateral interfacial engineering. <i>Journal of Catalysis</i> , 2021 , 404, 18-31	7.3	2
869	Dissociation of air pollutants on the uniform surface of pentagonal BeP ₂ . <i>Applied Surface Science</i> , 2021 , 570, 151061	6.7	0
868	Organic Batteries: the Route Toward Sustainable Electrical Energy Storage Technologies 2021 , 1-22		
867	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	5.5	2
866	Future Outlook and Direction of Next-Generation Battery Materials 2021 , 1-22		
865	Computational and Experimental Techniques to Envisage Battery Materials 2021 , 1-22		
864	MXene binder stabilizes pseudocapacitance of conducting polymers. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 20356-20361	13	1

863	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	13	3
862	Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. <i>Nanomaterials</i> , 2020 , 10,	5.4	5
861	Poisonous Vapor Adsorption on Pure and Modified Aluminum Nitride Nanosheet for Environmental Safety: A DFT Exploration. <i>Sustainability</i> , 2020 , 12, 10097	3.6	
860	Promising high-temperature thermoelectric response of bismuth oxybromide. <i>Results in Physics</i> , 2020 , 19, 103584	3.7	9
859	Highly Energetic and Stable Gadolinium/Bismuth Molybdate with a Fast Reactive Species, Redox Mechanism of Aqueous Electrolyte. <i>ACS Applied Energy Materials</i> , 2020 , 3, 12385-12399	6.1	6
858	Defective and doped aluminum nitride monolayers for NO adsorption: Physical insight. <i>Chemical Physics Letters</i> , 2020 , 753, 137592	2.5	3
857	Influence of Kubas-type interaction of B@Li codoped graphdiyne with hydrogen molecules on desorption temperature and storage efficiency. <i>Materials Today Energy</i> , 2020 , 16, 100421	7	2
856	Molecules versus Nanoparticles: Identifying a Reactive Molecular Intermediate in the Synthesis of Ternary Coinage Metal Chalcogenides. <i>Inorganic Chemistry</i> , 2020 , 59, 7727-7738	5.1	8
855	Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities. <i>Journal of Applied Physics</i> , 2020 , 127, 184305	2.5	9
854	Structural Phase Transitions, Electronic Properties, and Hardness of RuB ₄ under High Pressure in Comparison with FeB ₄ and OsB ₄ . <i>Journal of Physical Chemistry C</i> , 2020 , 124, 14804-14810	3.8	10
853	Hydrogen storage characteristics of Li and Na decorated 2D boron phosphide. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 4538-4546	5.8	21
852	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. <i>Science Advances</i> , 2020 , 6, eabb8097	14.3	97
851	Exploring the Possibility of BPhase Arsenic-Phosphorus Polymorph Monolayer as Anode Materials for Sodium-Ion Batteries. <i>Advanced Theory and Simulations</i> , 2020 , 3, 2000023	3.5	8
850	Effect of Cycling Ion and Solvent on the Redox Chemistry of Substituted Quinones and Solvent-Induced Breakdown of the Correlation between Redox Potential and Electron-Withdrawing Power of Substituents. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 13609-13617	3.8	12
849	Enhancement of hydrogen storage capacity on co-functionalized GaS monolayer under external electric field. <i>International Journal of Hydrogen Energy</i> , 2020 , 45, 12384-12393	6.7	12
848	Strain-Engineered Metal-Free h-B ₂ O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7884-7892	3.8	9
847	Capacity enhancement of polyolithiated functionalized boron nitride nanotubes: an efficient hydrogen storage medium. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15675-15682	3.6	5
846	High exothermic dissociation in van der Waals like hexagonal two dimensional nitrogene from first principles molecular dynamics. <i>Applied Surface Science</i> , 2020 , 529, 146552	6.7	7

845	Highly sensitive and selective sensing properties of modified green phosphorene monolayers towards SF ₆ decomposition gases. <i>Applied Surface Science</i> , 2020 , 512, 145641	6.7	16
844	Van der Waals induced molecular recognition of canonical DNA nucleobases on a 2D GaS monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 6706-6715	3.6	4
843	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 2363-2369	5.8	37
842	Rectifying behavior in twisted bilayer black phosphorus nanojunctions mediated through intrinsic anisotropy. <i>Nanoscale Advances</i> , 2020 , 2, 1493-1501	5.1	9
841	Room-temperature conversion of CuSe to CuAgSe nanoparticles to enhance the photocatalytic performance of their composites with TiO ₂ . <i>Dalton Transactions</i> , 2020 , 49, 3580-3591	4.3	9
840	Exploring two-dimensional M ₂ NS ₂ (M = Ti, V) MXenes based gas sensors for air pollutants. <i>Applied Materials Today</i> , 2020 , 19, 100574	6.6	20
839	HfS ₂ and TiS ₂ Monolayers with Adsorbed C, N, P Atoms: A First Principles Study. <i>Catalysts</i> , 2020 , 10, 94	4	1
838	The role of Ge ₂ Sb ₂ Te ₅ in enhancing the performance of functional plasmonic devices. <i>Materials Today Physics</i> , 2020 , 12, 100178	8	53
837	Nonlinear optical characteristics of an exciton in a GaSb-capped InSb heterodot: role of size control. <i>European Physical Journal Plus</i> , 2020 , 135, 1	3.1	2
836	Superior sensitivity of metal functionalized boron carbide (BC ₃) monolayer towards carbonaceous pollutants. <i>Applied Surface Science</i> , 2020 , 512, 145637	6.7	9
835	Crystallography of low Z material at ultrahigh pressure: Case study on solid hydrogen. <i>Matter and Radiation at Extremes</i> , 2020 , 5, 038401	4.7	11
834	Fluoride ion batteries: Designing flexible M ₂ CH ₂ (M=Ti or V) MXenes as high-capacity cathode materials. <i>Nano Energy</i> , 2020 , 74, 104911	17.1	17
833	Functionalized Two-Dimensional Nanoporous Graphene as Efficient Global Anode Materials for Li-, Na-, K-, Mg-, and Ca-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 9734-9745	3.8	17
832	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. <i>Nanoscale Advances</i> , 2020 , 2, 2410-2421	5.1	5
831	Interplay of charge density wave and multiband superconductivity in layered quasi-two-dimensional materials: The case of 2H-NbS ₂ and 2H-NbSe ₂ . <i>Physical Review Materials</i> , 2020 , 4,	3.2	15
830	Large pressure-induced magnetoresistance in a hybrid ferromagnet-semiconductor system: Effect of matrix modification on the spin-dependent scattering. <i>Journal of Applied Physics</i> , 2020 , 128, 213903	2.5	1
829	Carbon-phosphide monolayer with high carrier mobility and perceptible I _{ON} /I _{OFF} response for superior gas sensing. <i>New Journal of Chemistry</i> , 2020 , 44, 3777-3785	3.6	15
828	Superconductivity of superhydride CeH ₁₀ under high pressure. <i>Materials Research Express</i> , 2020 , 7, 086001	10.7	15

827	Progress in supercapacitors: roles of two dimensional nanotubular materials. <i>Nanoscale Advances</i> , 2020 , 2, 70-108	5.1	91
826	Orbital hybridization-induced band offset phenomena in NiCdO thin films. <i>Nanoscale</i> , 2020 , 12, 669-686	7.7	7
825	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	5.8	8
824	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C ₃ N ₄) nanosheets under selected transition metal doping. <i>International Journal of Hydrogen Energy</i> , 2020 , 45, 3035-3045	6.7	43
823	Boron-Rich Molybdenum Boride with Unusual Short-Range Vacancy Ordering, Anisotropic Hardness, and Superconductivity. <i>Chemistry of Materials</i> , 2020 , 32, 459-467	9.6	18
822	Terahertz plasmonics: The rise of toroidal metadvice towards immunobiosensings. <i>Materials Today</i> , 2020 , 32, 108-130	21.8	148
821	Insights into the trapping mechanism of light metals on C ₂ N-h ₂ D: Utilisation as an anode material for metal ion batteries. <i>Carbon</i> , 2020 , 160, 125-132	10.4	15
820	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. <i>Catalysts</i> , 2020 , 10, 1111	4	18
819	Improved Adsorption and Migration of Divalent Ions Over C ₄ N Nanosheets: Potential Anode for Divalent Batteries. <i>Surfaces and Interfaces</i> , 2020 , 21, 100758	4.1	3
818	Superior Anchoring of Sodium Polysulfides to the Polar CN 2D Material: A Potential Electrode Enhancer in Sodium-Sulfur Batteries. <i>Langmuir</i> , 2020 , 36, 13104-13111	4	11
817	Excitonic effects in the optoelectronic properties of graphene-like BC monolayer. <i>Optical Materials</i> , 2020 , 110, 110476	3.3	4
816	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	3.8	5
815	Tuning Hydrogen Storage Properties of Carbon Nanosheets through Selected Foreign Metal Functionalization. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 16827-16837	3.8	5
814	Bulk and monolayer As ₂ S ₃ as promising thermoelectric material with high conversion performance. <i>Computational Materials Science</i> , 2020 , 183, 109913	3.2	10
813	Rational Design of 2D h-BAs Monolayer as Advanced Sulfur Host for High Energy Density LiS Batteries. <i>ACS Applied Energy Materials</i> , 2020 , 3, 7306-7317	6.1	10
812	Impact of stacking on the optoelectronic properties of 2D ZrS ₂ /GaS heterostructure. <i>Materials Today: Proceedings</i> , 2020 , 47, 526-526	1.4	1
811	Core-shell nanostructures: perspectives towards drug delivery applications. <i>Journal of Materials Chemistry B</i> , 2020 ,	7.3	61
810	Emerging piezochromism in transparent lead free perovskite Rb ₃ X ₂ I ₉ (X = Sb, Bi) under compression: A comparative theoretical insight. <i>Journal of Applied Physics</i> , 2020 , 128, 045102	2.5	2

809	Reaction coordinate mapping of hydrogen evolution mechanism on Mg ₃ N ₂ monolayer. <i>International Journal of Hydrogen Energy</i> , 2020 , 45, 22848-22854	6.7	3
808	Ultrathin nanowire PdX ₂ (X = P, As): stability, electronic transport and thermoelectric properties. <i>New Journal of Chemistry</i> , 2020 , 44, 15617-15624	3.6	0
807	Turning indium oxide into high-performing electrode materials via cation substitution strategy: Preserving single crystalline cubic structure of 2D nanoflakes towards energy storage devices. <i>Journal of Power Sources</i> , 2020 , 480, 228873	8.9	33
806	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS ₃ (A = Mg, Ca, Sr and Ba) under pressure. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 16392-16403	7.1	9
805	Route to high-[Formula: see text] superconductivity of [Formula: see text] via strong bonding of boron-carbon compound at high pressure. <i>Scientific Reports</i> , 2020 , 10, 18090	4.9	9
804	Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. <i>ChemCatChem</i> , 2020 , 12, 6013-6023	5.2	12
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