

Deobrat Singh

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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.

93
papers

1,135
citations

18
h-index

30
g-index

108
ext. papers

1,644
ext. citations

5.1
avg, IF

5.3
L-index

#	Paper	IF	Citations
93	Antimonene: a monolayer material for ultraviolet optical nanodevices. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 6386-6390	7.1	178
92	2D-HfS ₂ as an efficient photocatalyst for water splitting. <i>Catalysis Science and Technology</i> , 2016 , 6, 6605-6614	5.14	52
91	Efficient and selective sensing of nitrogen-containing gases by Si ₂ BN nanosheets under pristine and pre-oxidized conditions. <i>Applied Surface Science</i> , 2019 , 469, 775-780	6.7	47
90	Necklace-like Nitrogen-Doped Tubular Carbon 3D Frameworks for Electrochemical Energy Storage. <i>Advanced Functional Materials</i> , 2020 , 30, 1909725	15.6	46
89	Germanene: a new electronic gas sensing material. <i>RSC Advances</i> , 2016 , 6, 102264-102271	3.7	46
88	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 12312-12320	7.1	45
87	Sensing of volatile organic compounds on two-dimensional nitrogenated holey graphene, graphdiyne, and their heterostructure. <i>Carbon</i> , 2020 , 163, 213-223	10.4	38
86	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 2363-2369	5.8	37
85	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (= Se and Te). <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 46212-46219	9.5	35
84	High performance material for hydrogen storage: Graphenelike Si ₂ BN solid. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 22942-22952	6.7	33
83	Single layer of carbon phosphide as an efficient material for optoelectronic devices. <i>Journal of Materials Science</i> , 2018 , 53, 8314-8327	4.3	32
82	Novel green phosphorene as a superior chemical gas sensing material. <i>Journal of Hazardous Materials</i> , 2021 , 401, 123340	12.8	32
81	Indiene 2D monolayer: a new nanoelectronic material. <i>RSC Advances</i> , 2016 , 6, 8006-8014	3.7	30
80	Impact of edge structures on interfacial interactions and efficient visible-light photocatalytic activity of metal/semiconductor hybrid 2D materials. <i>Catalysis Science and Technology</i> , 2020 , 10, 3279-3289	5.5	24
79	Two-Dimensional CH ₃ NH ₃ PbI ₃ with High Efficiency and Superior Carrier Mobility: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 5231-5239	3.8	23
78	Experimental and theoretical analysis of electronic and optical properties of MgWO ₄ . <i>Journal of Materials Science</i> , 2017 , 52, 4934-4943	4.3	19
77	Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional SiBN. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 21716-21723	3.6	18

76	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. <i>Catalysts</i> , 2020 , 10, 1111	4	18
75	Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping. <i>Nanotechnology</i> , 2017 , 28, 495202	3.4	17
74	First step to investigate nature of electronic states and transport in flower-like MoS ₂ : Combining experimental studies with computational calculations. <i>Scientific Reports</i> , 2016 , 6, 32690	4.9	17
73	Enhanced Optoelectronic and Thermoelectric Properties by Intrinsic Structural Defects in Monolayer HfS ₂ . <i>ACS Applied Energy Materials</i> , 2019 , 2, 6891-6903	6.1	17
72	Carbon-phosphide monolayer with high carrier mobility and perceptible I _V response for superior gas sensing. <i>New Journal of Chemistry</i> , 2020 , 44, 3777-3785	3.6	15
71	Recent progress of defect chemistry on 2D materials for advanced battery anodes. <i>Chemistry - an Asian Journal</i> , 2020 , 15, 3390-3404	4.5	15
70	Sensing the polar molecules MH ₃ (M = N, P, or As) with a Janus NbTeSe monolayer. <i>New Journal of Chemistry</i> , 2020 , 44, 7932-7940	3.6	15
69	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
68	Optical excitations and thermoelectric properties of two-dimensional holey graphene. <i>Physical Review B</i> , 2020 , 102,	3.3	12
67	Improving electron transport in the hybrid perovskite solar cells using CaMnO ₃ -based buffer layer. <i>Nano Energy</i> , 2018 , 45, 287-297	17.1	11
66	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
65	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
64	Density functional Studies of structural, electronic and vibrational properties of palladium oxide. <i>Solid State Communications</i> , 2016 , 245, 36-41	1.6	10
63	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. <i>Applied Surface Science</i> , 2021 , 556, 149561	6.7	10
62	MgF ₂ monolayer as an anti-reflecting material. <i>Solid State Communications</i> , 2017 , 252, 22-28	1.6	9
61	Promising high-temperature thermoelectric response of bismuth oxybromide. <i>Results in Physics</i> , 2020 , 19, 103584	3.7	9
60	Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities. <i>Journal of Applied Physics</i> , 2020 , 127, 184305	2.5	9
59	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

58	Room-temperature conversion of CuSe to CuAgSe nanoparticles to enhance the photocatalytic performance of their composites with TiO. <i>Dalton Transactions</i> , 2020 , 49, 3580-3591	4.3	9
57	Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices. <i>Scientific Reports</i> , 2019 , 9, 17300	4.9	9
56	Emergence of Si2BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. <i>ACS Applied Energy Materials</i> , 2019 , 2, 8441-8448	6.1	9
55	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
54	High temperature-mediated rocksalt to wurtzite phase transformation in cadmium oxide nanosheets and its theoretical evidence. <i>Nanoscale</i> , 2019 , 11, 14802-14819	7.7	8
53	2D g-C3N4 monolayer for amino acids sequencing. <i>Applied Surface Science</i> , 2020 , 528, 146609	6.7	7
52	Harnessing the unique properties of MXenes for advanced rechargeable batteries. <i>JPhys Energy</i> , 2021 , 3, 012005	4.9	7
51	Orbital hybridization-induced band offset phenomena in NiCdO thin films. <i>Nanoscale</i> , 2020 , 12, 669-686	7.7	7
50	The influence of edge structure on the optoelectronic properties of Si2BN quantum dot. <i>Journal of Applied Physics</i> , 2019 , 126, 233104	2.5	7
49	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
48	Electronic, Magnetic and Optical Properties of 2D Metal Nanolayers: A DFT Study. <i>Metals and Materials International</i> , 2018 , 24, 904-912	2.4	6
47	Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. <i>Nanomaterials</i> , 2020 , 10,	5.4	5
46	Two-dimensional Nitrogenated Holey Graphene (C2N) monolayer based glucose sensor for diabetes mellitus. <i>Applied Surface Science</i> , 2022 , 573, 151579	6.7	5
45	Structural and electrical properties of CeO2 monolayers using first-principles calculations. <i>Solid State Communications</i> , 2020 , 307, 113801	1.6	5
44	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
43	Cobalt tetrphosphate as an efficient bifunctional electrocatalyst for hybrid sodium-air batteries. <i>Nano Energy</i> , 2021 , 89, 106485	17.1	5
42	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
41	Spin-entropy induced thermopower and spin-blockade effect in CoO. <i>Physical Review B</i> , 2019 , 100,	3.3	4

40	Excitonic effects in the optoelectronic properties of graphene-like BC monolayer. <i>Optical Materials</i> , 2020 , 110, 110476	3.3	4
39	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
38	Effect of oxygen atom on electronic and optical properties of 2D monolayer of PtS ₂ 2017 ,		3
37	Ab Initio Investigation of Vibrational, Optical and Thermodynamics Properties of Yttrium Arsenide. <i>Journal of Electronic Materials</i> , 2017 , 46, 5670-5676	1.9	3
36	Structural, vibrational and optoelectronic properties of buckled metallic FeGe monolayer. <i>Superlattices and Microstructures</i> , 2019 , 129, 62-68	2.8	3
35	Effect on electronic and optical properties of Frenkel and Schottky defects in HfS ₂ monolayer 2018 ,		3
34	Theoretical Prediction of a Bi-Doped β Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56254-56264	9.5	3
33	Temperature-Dependent Cationic Doping-Driven Phonon Dynamics Investigation in CdO Thin Films Using Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 21818-21828	3.8	3
32	Dimensionality effects in high-performance thermoelectric materials: Computational and experimental progress in energy harvesting applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , e1547	7.9	3
31	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
30	Study of air stability mechanism of 2D boron antimonide 2019 ,		2
29	Temperature and Size Dependent Thermal Conductivity of Graphene Nanoribbons Description for Phonon Dispersion and Polarization. <i>Advanced Science Letters</i> , 2016 , 22, 3916-3918	0.1	2
28	First-principles study of the electronic, magnetic and optical properties of Fe ₃ Se ₄ in its monoclinic phase. <i>Journal of Magnetism and Magnetic Materials</i> , 2020 , 498, 166157	2.8	2
27	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
26	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
25	Structural, electronic and ferroelectric properties of BaTcO ₃ 2017 ,		1
24	Effect on electronic, optical and transport properties of Cu ₂ O and Au doped Cu ₂ O: A DFT investigation 2019 ,		1
23	2D monolayer boron sulfide as an efficient material for optical nanodevices 2020 ,		1

22	Metal-Mott insulator transition of SrMnO ₃ by fluorine doping 2017 ,		1
21	Structural, electronic and ferroelectric properties of BaReO ₃ 2017 ,		1
20	Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solid-liquid interfaces. <i>Nanoscale Advances</i> , 2022 , 4, 884-893	5.1	1
19	2D MgF ₂ nanosheet as a promising candidate for thermoelectric material. <i>Materials Today: Proceedings</i> , 2020 ,	1.4	1
18	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
17	Structural and opto-electronic properties of 2D AlSb monolayer 2016 ,		1
16	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
15	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
14	Catalyzing Bond-Dissociation in Graphene via Alkali-Iodide Molecules. <i>Small</i> , 2021 , 17, e2102037	11	1
13	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
12	Bifunctional Catalytic Activity of 2D Boron Monochalcogenides BX (X = S, Se, Te). <i>Materials Today Energy</i> , 2022 , 101026	7	1
11	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. <i>Crystal Growth and Design</i> ,	3.5	0
10	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
9	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
8	Correlation between reduced dielectric loss and charge migration kinetics in NdFeO ₃ -modified Ba _{0.7} Sr _{0.3} TiO ₃ ceramics. <i>Journal of Materials Science: Materials in Electronics</i> , 2021 , 32, 24910	2.1	0
7	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
6	Vibrational Properties of Zr-Ni Metallic Glasses. <i>Materials Today: Proceedings</i> , 2016 , 3, 3137-3143	1.4	
5	Van der Waals Heterostructure-Based Anode Materials 2021 , 1-18		

4 Introduction: Background of Computational and Experimental Investigations for Next-Generation Efficient Battery Materials **2021**, 1-34

3 Graphene-Based Anode Materials for Li and Na Batteries **2021**, 1-24

2 Coexisting commensurate and incommensurate charge ordered phases in CoO. *Scientific Reports*, **2021**, 11, 19415 4-9

1 Organic Batteries: the Route Toward Sustainable Electrical Energy Storage Technologies **2021**, 1-22