Deobrat Singh

List of Publications by Year
in descending order

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106 papers	2,244 citations	236912 25 h-index	265191 42 g-index
108 all docs	108 docs citations	108 times ranked	1980 citing authors

#	Article	IF	Citations
1	Dimensionality effects in highâ€performance thermoelectric materials: Computational and experimental progress in energy harvesting applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1547.	14.6	20
2	Two-dimensional Nitrogenated Holey Graphene (C2N) monolayer based glucose sensor for diabetes mellitus. Applied Surface Science, 2022, 573, 151579.	6.1	20
3	Asymmetry-Induced Redistribution in Sn(IV)â€“Ti(IV) Hetero-Bimetallic Alkoxide Precursors and Its Impact on Thin-Film Deposition by Metalâ€“Organic Chemical Vapor Deposition. Crystal Growth and Design, 2022, 22, 54-59.	3.0	1
4	First-principles calculations to investigate electronic structure and optical properties of 2D MgCl2 monolayer. Superlattices and Microstructures, 2022, 162, 107132.	3.1	15
5	Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solidâ€“liquid interfaces. Nanoscale Advances, 2022, 4, 884-893.	4.6	4
6	Two-Dimensional Perovskite/HfS₂ van der Waals Heterostructure as an Absorber Material for Photovoltaic Applications. ACS Applied Energy Materials, 2022, 5, 2300-2307.	5.1	9
7	Exotic magnetic and electronic properties of layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn></mml:msub></m single crystals under high pressure. Physical Review B, 2022, 105, .	3.2	12
8	2D Janus and non-Janus diamanes with an in-plane negative Poisson's ratio for energy applications. Materials Today Advances, 2022, 14, 100225.	5.2	10
9	Janus Aluminum Oxysulfide Al2OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. Applied Surface Science, 2022, 589, 152997.	6.1	21
10	Activationâ€Induced Surface Modulation of Biowasteâ€Derived Hierarchical Porous Carbon for Supercapacitors. ChemPlusChem, 2022, 87, .	2.8	18
11	Bifunctional catalytic activity of 2D boron monochalcogenides BX (XÂ=ÂS, Se, Te). Materials Today Energy, 2022, 27, 101026.	4.7	7
12	Flexible 3D porous boron nitride interconnected network as a high-performance Li-and Na-ion battery electrodes. Electrochimica Acta, 2022, 421, 140491.	5.2	9
13	Probing the electronic, optical and transport properties of halide double perovskites Rb2InSb(Cl,Br)6 for solar cells and thermoelectric applications. Journal of Solid State Chemistry, 2022, 312, 123262.	2.9	10
14	Optoelectronic properties of 2D van der Waals heterostructure As/PtS2 by first-principles calculations. Materials Today: Proceedings, 2022, 67, 250-253.	1.8	1
15	Impact of stacking on the optoelectronic properties of 2D ZrS2/GaS heterostructure. Materials Today: Proceedings, 2021, 47, 526-528.	1.8	9
16	Novel green phosphorene as a superior chemical gas sensing material. Journal of Hazardous Materials, 2021, 401, 123340.	12.4	71
17	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
18	Mechanism of formaldehyde and formic acid formation on (101)-TiO₂@Cu₄ systems through CO₂ hydrogenation. Sustainable Energy and Fuels, 2021, 5, 564-574.	4.9	4

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19	Van der Waals Heterostructure-Based Anode Materials. , 2021, , 1-18.		0
20	Introduction: Background of Computational and Experimental Investigations for Next-Generation Efficient Battery Materials. , 2021, , 1-34.		0
21	Hydrogenation and oxidation enhances the thermoelectric performance of Si₂BN monolayer. New Journal of Chemistry, 2021, 45, 3892-3900.	2.8	8
22	Graphene-Based Anode Materials for Li and Na Batteries. , 2021, , 1-24.		0
23	Antimonene Allotropes Î±- and Î²-Phases as Promising Anchoring Materials for Lithiumâ€"Sulfur Batteries. Energy & Fuels, 2021, 35, 9001-9009.	5.1	15
24	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. Applied Surface Science, 2021, 556, 149561.	6.1	31
25	High-Specific-Capacity and High-Performing Post-Lithium-Ion Battery Anode over 2D Black Arsenic Phosphorus. ACS Applied Energy Materials, 2021, 4, 7900-7910.	5.1	19
26	Correlation between reduced dielectric loss and charge migration kinetics in NdFeO3-modified Ba0.7Sr0.3TiO3 ceramics. Journal of Materials Science: Materials in Electronics, 2021, 32, 24910.	2.2	2
27	Catalyzing Bondâ€Dissociation in Graphene via Alkaliâ€Iodide Molecules. Small, 2021, 17, e2102037.	10.0	1
28	Coexisting commensurate and incommensurate charge ordered phases in CoO. Scientific Reports, 2021, 11, 19415.	3.3	0
29	Cobalt tetraphosphate as an efficient bifunctional electrocatalyst for hybrid sodium-air batteries. Nano Energy, 2021, 89, 106485.	16.0	11
30	Organic Batteries: the Route Toward Sustainable Electrical Energy Storage Technologies. , 2021, , 1-22.		2
31	Influence of vacancy and adatom defects on the optoelectronic properties of monolayer GeS. AIP Conference Proceedings, 2021, , .	0.4	0
32	Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications. Catalysis Science and Technology, 2021, 11, 4996-5013.	4.1	18
33	Harnessing the unique properties of MXenes for advanced rechargeable batteries. JPhys Energy, 2021, 3, 012005.	5.3	14
34	Polypeptoid Material as an Anchoring Material for Liâ€"S Batteries. ACS Applied Energy Materials, 2021, 4, 13070-13076.	5.1	8
35	Theoretical Prediction of a Bi-Doped Î²-Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. ACS Applied Materials & Interfaces, 2021, 13, 56254-56264.	8.0	10
36	First-principles study of the electronic, magnetic and optical properties of Fe3Se4 in its monoclinic phase. Journal of Magnetism and Magnetic Materials, 2020, 498, 166157.	2.3	6

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37	Orbital hybridization-induced band offset phenomena in Ni_xCd_{1â^'x}O thin films. Nanoscale, 2020, 12, 669-686.	5.6	11
38	Structural and electrical properties of CeO2 monolayers using first-principles calculations. Solid State Communications, 2020, 307, 113801.	1.9	12
39	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. Catalysts, 2020, 10, 1111.	3.5	35
40	Excitonic effects in the optoelectronic properties of graphene-like BC monolayer. Optical Materials, 2020, 110, 110476.	3.6	19
41	Bulk and monolayer As2S3 as promising thermoelectric material with high conversion performance. Computational Materials Science, 2020, 183, 109913.	3.0	24
42	Rational Design of 2D h-BAs Monolayer as Advanced Sulfur Host for High Energy Density Liâ€"S Batteries. ACS Applied Energy Materials, 2020, 3, 7306-7317.	5.1	23
43	2D MgF2 nanosheet as a promising candidate for thermoelectric material. Materials Today: Proceedings, 2020, , .	1.8	1
44	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
45	Optical excitations and thermoelectric properties of two-dimensional holey graphene. Physical Review B, 2020, 102, .	3.2	28
46	Recent progress of defect chemistry on 2D materials for advanced battery anodes. Chemistry - an Asian Journal, 2020, 15, 3390-3404.	3.3	35
47	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (X = Se) Tj ETQq1 1 0.784314 rgBT /Overl	8.0	130
48	Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. Nanomaterials, 2020, 10, 2554.	4.1	17
49	Promising high-temperature thermoelectric response of bismuth oxybromide. Results in Physics, 2020, 19, 103584.	4.1	27
50	Highly Energetic and Stable Gadolinium/Bismuth Molybdate with a Fast Reactive Species, Redox Mechanism of Aqueous Electrolyte. ACS Applied Energy Materials, 2020, 3, 12385-12399.	5.1	21
51	Revealing the veil of the stability of monolayer boron sulfide upon air and humidity exposure. AIP Conference Proceedings, 2020, , .	0.4	0
52	Molecules versus Nanoparticles: Identifying a Reactive Molecular Intermediate in the Synthesis of Ternary Coinage Metal Chalcogenides. Inorganic Chemistry, 2020, 59, 7727-7738.	4.0	10
53	Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities. Journal of Applied Physics, 2020, 127, .	2.5	19
54	2D g-C3N4 monolayer for amino acids sequencing. Applied Surface Science, 2020, 528, 146609.	6.1	11

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55	Enhancement of hydrogen storage capacity on co-functionalized GaS monolayer under external electric field. International Journal of Hydrogen Energy, 2020, 45, 12384-12393.	7.1	24
56	Strain-Engineered Metal-Free h-B₂O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 7884-7892.	3.1	27
57	Sensing of volatile organic compounds on two-dimensional nitrogenated holey graphene, graphdiyne, and their heterostructure. Carbon, 2020, 163, 213-223.	10.3	77
58	2D monolayer boron sulfide as an efficient material for optical nanodevices. AIP Conference Proceedings, 2020, , .	0.4	2
59	Electronic and optical properties of a structural defect in 2D MgF2 monolayer. AIP Conference Proceedings, 2020, , .	0.4	4
60	Van der Waals induced molecular recognition of canonical DNA nucleobases on a 2D GaS monolayer. Physical Chemistry Chemical Physics, 2020, 22, 6706-6715.	2.8	5
61	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. Sustainable Energy and Fuels, 2020, 4, 2363-2369.	4.9	62
62	Room-temperature conversion of Cu_{2â^'x}Se to CuAgSe nanoparticles to enhance the photocatalytic performance of their composites with TiO₂. Dalton Transactions, 2020, 49, 3580-3591.	3.3	13
63	Necklaceâ€like Nitrogenâ€Doped Tubular Carbon 3D Frameworks for Electrochemical Energy Storage. Advanced Functional Materials, 2020, 30, 1909725.	14.9	89
64	Impact of edge structures on interfacial interactions and efficient visible-light photocatalytic activity of metalâ€"semiconductor hybrid 2D materials. Catalysis Science and Technology, 2020, 10, 3279-3289.	4.1	37
65	Sensing the polar molecules MH3 (M = N, P, or As) with a Janus NbTeSe monolayer. New Journal of Chemistry, 2020, 44, 7932-7940.	2.8	20
66	Carbon-phosphide monolayer with high carrier mobility and perceptibleIâ€"Vresponse for superior gas sensing. New Journal of Chemistry, 2020, 44, 3777-3785.	2.8	23
67	Enhanced Optoelectronic and Thermoelectric Properties by Intrinsic Structural Defects in Monolayer HfS₂. ACS Applied Energy Materials, 2019, 2, 6891-6903.	5.1	31
68	High temperature-mediated rocksalt to wurtzite phase transformation in cadmium oxide nanosheets and its theoretical evidence. Nanoscale, 2019, 11, 14802-14819.	5.6	15
69	Ab-initio study of strain engineering optical properties of RbPbI3. AIP Conference Proceedings, 2019, , .	0.4	2
70	Study of stability of 2D boron arsenide in air at atomic level. AIP Conference Proceedings, 2019, , .	0.4	0
71	Spin-entropy induced thermopower and spin-blockade effect in CoO. Physical Review B, 2019, 100, .	3.2	6
72	Study of air stability mechanism of 2D boron antimonide. AIP Conference Proceedings, 2019, , .	0.4	2

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73	Effect on electronic, optical and transport properties of Cu2O and Au doped Cu2O: A DFT investigation. AIP Conference Proceedings, 2019, , .	0.4	1
74	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. Journal of Materials Chemistry C, 2019, 7, 12312-12320.	5.5	85
75	Structural, vibrational and optoelectronic properties of buckled metallic FeGe monolayer. Superlattices and Microstructures, 2019, 129, 62-68.	3.1	3
76	Two-Dimensional CH₃NH₃PbI₃ with High Efficiency and Superior Carrier Mobility: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 5231-5239.	3.1	41
77	The influence of edge structure on the optoelectronic properties of Si2BN quantum dot. Journal of Applied Physics, 2019, 126, .	2.5	17
78	Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices. Scientific Reports, 2019, 9, 17300.	3.3	18
79	Emergence of Si₂BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. ACS Applied Energy Materials, 2019, 2, 8441-8448.	5.1	18
80	Efficient and selective sensing of nitrogen-containing gases by Si2BN nanosheets under pristine and pre-oxidized conditions. Applied Surface Science, 2019, 469, 775-780.	6.1	78
81	Single layer of carbon phosphide as an efficient material for optoelectronic devices. Journal of Materials Science, 2018, 53, 8314-8327.	3.7	41
82	Effect on electronic and optical properties of Frenkel and Schottky defects in HfS2 monolayer. AIP Conference Proceedings, 2018, , .	0.4	5
83	Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer. Nano Energy, 2018, 45, 287-297.	16.0	19
84	Electronic, Magnetic and Optical Properties of 2D Metal Nanolayers: A DFT Study. Metals and Materials International, 2018, 24, 904-912.	3.4	6
85	Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional Si₂BN. Physical Chemistry Chemical Physics, 2018, 20, 21716-21723.	2.8	30
86	MgF 2 monolayer as an anti-reflecting material. Solid State Communications, 2017, 252, 22-28.	1.9	27
87	Structural, electronic and ferroelectric properties of BaTcO3. AIP Conference Proceedings, 2017, , .	0.4	1
88	Electronic and transport properties of fluorite structure of La2Ce2O7. AIP Conference Proceedings, 2017, , .	0.4	1
89	Effect of oxygen atom on electronic and optical properties of 2D monolayer of PtS2. AIP Conference Proceedings, 2017, , .	0.4	4
90	Ab Initio Investigation of Vibrational, Optical and Thermodynamics Properties of Yttrium Arsenide. Journal of Electronic Materials, 2017, 46, 5670-5676.	2.2	4

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91	Experimental and theoretical analysis of electronic and optical properties of MgWO4. Journal of Materials Science, 2017, 52, 4934-4943.	3.7	28
92	Modulating the electronic and optical properties of monolayer arsenene phases by organic molecular doping. Nanotechnology, 2017, 28, 495202.	2.6	22
93	Metal-Mott insulator transition of SrMnO3 by fluorine doping. AIP Conference Proceedings, 2017, , .	0.4	1
94	High performance material for hydrogen storage: Graphenelike Si2BN solid. International Journal of Hydrogen Energy, 2017, 42, 22942-22952.	7.1	50
95	Structural, electronic and ferroelectric properties of BaReO3. AIP Conference Proceedings, 2017, , .	0.4	2
96	Density functional Studies of structural, electronic and vibrational properties of palladium oxide. Solid State Communications, 2016, 245, 36-41.	1.9	13
97	Vibrational Properties of Zrâ€"Ni Metallic Glasses. Materials Today: Proceedings, 2016, 3, 3137-3143.	1.8	0
98	First-principles study of structural & electronic properties of pyramidal silicon nanowire. AIP Conference Proceedings, 2016, , .	0.4	3
99	Structural and opto-electronic properties of 2D AlSb monolayer. AIP Conference Proceedings, 2016, , .	0.4	2
100	Germanene: a new electronic gas sensing material. RSC Advances, 2016, 6, 102264-102271.	3.6	68
101	First step to investigate nature of electronic states and transport in flower-like MoS2: Combining experimental studies with computational calculations. Scientific Reports, 2016, 6, 32690.	3.3	20
102	Mechanical properties of 4d transition metals in molten state. AIP Conference Proceedings, 2016, , .	0.4	0
103	Antimonene: a monolayer material for ultraviolet optical nanodevices. Journal of Materials Chemistry C, 2016, 4, 6386-6390.	5.5	246
104	2D-HfS₂as an efficient photocatalyst for water splitting. Catalysis Science and Technology, 2016, 6, 6605-6614.	4.1	71
105	Indiene 2D monolayer: a new nanoelectronic material. RSC Advances, 2016, 6, 8006-8014.	3.6	45
106	Temperature and Size Dependent Thermal Conductivity of Graphene Nanoribbons Description for Phonon Dispersion and Polarization. Advanced Science Letters, 2016, 22, 3916-3918.	0.2	2