

Ranjit Thapa

List of Publications by Year in descending order

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123
papers

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citations

134610

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123
all docs

123
docs citations

123
times ranked

6070
citing authors

#	ARTICLE	IF	CITATIONS
1	Origin of pure and C doped borophene stability and its activity for OER. Applied Surface Science, 2022, 574, 151613.	3.1	9
2	Understanding the role of lithium bonds in doped graphene nanoribbons as cathode hosts for Li^{\oplus} batteries: A first-principles study. International Journal of Energy Research, 2022, 46, 4405-4416.	2.2	8
3	Nanoribbons of 2D materials: A review on emerging trends, recent developments and future perspectives. Coordination Chemistry Reviews, 2022, 453, 214335.	9.5	20
4	First-principles identification of interface effect on Li storage capacity of C ₃ N/graphene multilayer heterostructure. Journal of Colloid and Interface Science, 2022, 610, 80-88.	5.0	11
5	Improved Oxygen Redox Activity by High-Valent Fe and Co ³⁺ Sites in the Perovskite LaNi _{1-x} Fe _{0.5x} Co _{0.5x} O ₃ . ACS Applied Energy Materials, 2022, 5, 343-354.	2.5	18
6	Structural Metamorphosis and Band Dislocation of Trirutile NiTa ₂ O ₆ under Compression. Journal of Physical Chemistry C, 2022, 126, 4106-4117.	1.5	1
7	Quasi-one-dimensional van der Waals TiS ₃ nanosheets for energy storage applications: Theoretical predications and experimental validation. Applied Physics Letters, 2022, 120, .	1.5	11
8	Low-Basis Weight Polyacrylonitrile/Polyvinylpyrrolidone Blend Nanofiber Membranes for Efficient Particulate Matter Capture. ACS Applied Polymer Materials, 2022, 4, 3971-3981.	2.0	7
9	Strategic Modulation of Target-Specific Isolated Fe,Co Single-Atom Active Sites for Oxygen Electrocatalysis Impacting High Power Zn-Air Battery. ACS Nano, 2022, 16, 7890-7903.	7.3	91
10	A Unique Bridging Facet Assembly of Gold Nanorods for the Detection of Thiram through Surface-Enhanced Raman Scattering. ACS Sustainable Chemistry and Engineering, 2022, 10, 7330-7340.	3.2	13
11	Understanding the Site-Selective Electrocatalytic Co-Reduction Mechanism for Green Urea Synthesis Using Copper Phthalocyanine Nanotubes. Advanced Functional Materials, 2022, 32, .	7.8	70
12	Low-Temperature Spin-Canted Magnetism and Bipolaron Freezing Electrical Transition in Potential Electron Field Emitter NdNiO ₃ . ACS Applied Electronic Materials, 2022, 4, 3134-3146.	2.0	3
13	Hydrogen-Bonded Organic Framework Structure: A Metal-Free Electrocatalyst for the Evolution of Hydrogen. ACS Omega, 2022, 7, 22440-22446.	1.6	5
14	Synergetic effect of localized and delocalized π electron on Li storage properties of Si/C heterostructures. Carbon, 2021, 171, 257-264.	5.4	7
15	Cu ₂ O/CuO heterojunction catalysts through atmospheric pressure plasma induced defect passivation. Applied Surface Science, 2021, 541, 148571.	3.1	43
16	Synthesis of CTAB-Functionalized Large-Scale Nanofibers Air Filter Media for Efficient PM _{2.5} Capture Capacity with Low Airflow Resistance. ACS Applied Polymer Materials, 2021, 3, 937-948.	2.0	20
17	Charge trapping characteristics of sputter-AlO _x /ALD Al ₂ O ₃ /Epitaxial-GaAs-based non-volatile memory. Journal of Materials Science: Materials in Electronics, 2021, 32, 4157-4165.	1.1	2
18	Novel Carbene Anchored Molecular Catalysts for Hydrogen Evolution Reactions. Journal of Physical Chemistry C, 2021, 125, 3793-3803.	1.5	10

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19	Scalable Production of Cobalt Phthalocyanine Nanotubes: Efficient and Robust Hollow Electrocatalyst for Ammonia Synthesis at Room Temperature. ACS Nano, 2021, 15, 5230-5239.	7.3	76
20	Controlled Loading of MoS ₂ on Hierarchical Porous TiO ₂ for Enhanced Photocatalytic Hydrogen Evolution. Journal of Physical Chemistry C, 2021, 125, 11950-11962.	1.5	40
21	Promoting reactivity of graphene based catalysts to achieve LH mechanism for CO oxidation. Catalysis Today, 2021, 370, 142-150.	2.2	8
22	Stable and boosted oxygen evolution efficiency of mixed metal oxide and borate planner heterostructure over heteroatom (N) doped electrochemically exfoliated graphite foam. Catalysis Today, 2021, 370, 83-92.	2.2	4
23	Advanced catalyst. Catalysis Today, 2021, 370, 1.	2.2	0
24	One-pot solvothermal synthesis of Co ₂ P nanoparticles: An efficient HER and OER electrocatalysts. International Journal of Hydrogen Energy, 2021, 46, 21924-21938.	3.8	60
25	Energy parameter and electronic descriptor for carbon based catalyst predicted using QM/ML. Applied Catalysis B: Environmental, 2021, 286, 119866.	10.8	23
26	Computationally exploring the role of S-dopant and S-linker in activating the catalytic efficiency of graphene quantum dot for ORR. Catalysis Today, 2021, 370, 36-45.	2.2	7
27	Nitrogen doping derived bridging of graphene and carbon nanotube composite for oxygen electroreduction. International Journal of Energy Research, 2021, 45, 21293-21306.	2.2	6
28	Nitrogen vacancy and hydrogen substitution mediated tunable optoelectronic properties of g-C ₃ N ₄ 2D layered structures: Applications towards blue LED to broad-band photodetection. Applied Surface Science, 2021, 556, 149773.	3.1	14
29	Enhanced energy storage performance and theoretical studies of 3D cuboidal manganese diselenides embedded with multiwalled carbon nanotubes. Journal of Colloid and Interface Science, 2021, 598, 500-510.	5.0	31
30	Metal-Free Triazine-Based 2D Covalent Organic Framework for Efficient H ₂ Evolution by Electrochemical Water Splitting. ChemSusChem, 2021, 14, 5057-5064.	3.6	42
31	Unveiling the genesis of the high catalytic activity in nickel phthalocyanine for electrochemical ammonia synthesis. Journal of Materials Chemistry A, 2021, 9, 14477-14484.	5.2	46
32	Ternary VS ₂ /ZnS/CdS hybrids as efficient electrocatalyst for hydrogen evolution reaction: Experimental and theoretical insights. AIP Advances, 2021, 11, .	0.6	13
33	Design principle of MoS ₂ /C heterostructure to enhance the quantum capacitance for supercapacitor application. Journal of Energy Storage, 2021, 44, 103476.	3.9	22
34	Structural, dielectric, electrical properties of Nd doped double perovskite ceramics and variation of density of states upon doping. Materials Chemistry and Physics, 2020, 239, 122250.	2.0	18
35	Microporous networks of NiMn ₂ O ₄ as a potent cathode material for electric field emission. Journal Physics D: Applied Physics, 2020, 53, 055103.	1.3	11
36	Role of van der Waals interaction in enhancing the photon absorption capability of the MoS ₂ /2D heterostructure. Physical Chemistry Chemical Physics, 2020, 22, 2775-2782.	1.3	5

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37	Fowlerâ€™Nordheim Law Correlated with Improved Field Emission in Selfâ€™Assembled NiCr ₂ O ₄ Nanosheets. Physica Status Solidi (A) Applications and Materials Science, 2020, 217, 1900741.	0.8	6
38	Dendritic Ferroselite (FeSe ₂) with 2D Carbon-Based Nanosheets of rGO and g-C ₃ N ₄ as Efficient Catalysts for Electrochemical Hydrogen Evolution. ACS Applied Energy Materials, 2020, 3, 12682-12691.	2.5	33
39	Pressure-induced octahedral tilting distortion and structural phase transition in columbite structured NiNb ₂ O ₆ . Journal of Applied Physics, 2020, 128, .	1.1	9
40	2D/3D heterostructure of h-BN/reduced graphite oxide as a remarkable electrode Material for supercapacitor. Journal of Power Sources, 2020, 479, 229092.	4.0	34
41	Defect-Engineered MoO ₂ Nanostructures as an Efficient Electrocatalyst for Oxygen Evolution Reaction. ACS Applied Energy Materials, 2020, 3, 5208-5218.	2.5	54
42	CO oxidation on Pt based binary and ternary alloy nanocatalysts: Reaction pathways and electronic descriptor. Applied Surface Science, 2020, 528, 146964.	3.1	14
43	B ₂ H ₆ splitting on catalytic surfaces and role of BH ₃ towards hydrogen spillover. Journal of Power Sources, 2020, 455, 227973.	4.0	2
44	Superior field emission and alternating current conduction mechanisms for grains and grain boundaries in an NiO-[CdO] ₂ nanocomposite. Journal of Physics and Chemistry of Solids, 2020, 142, 109462.	1.9	16
45	Electric field emission and anomalies of electrical conductivity above room temperature in heterogeneous NiO-SnO ₂ nano-ceramic composites. Journal of Applied Physics, 2020, 127, .	1.1	24
46	Stress-Induced Electronic Structure Modulation of Manganese-Incorporated Ni ₂ P Leading to Enhanced Activity for Water Splitting. ACS Applied Energy Materials, 2020, 3, 1271-1278.	2.5	24
47	Carbon Allotropes as Anode Material for Lithiumâ€™on Batteries. Advanced Materials Technologies, 2019, 4, 1900307.	3.0	50
48	First-principles identification of the origin for higher activity of surface doped carbon nanohorn: Impact on hydrogen storage. International Journal of Hydrogen Energy, 2019, 44, 23196-23209.	3.8	10
49	Screening of suitable cationic dopants for solar absorber material CZTS/Se: A first principles study. Scientific Reports, 2019, 9, 15983.	1.6	32
50	Core-composite mediated separation of diverse nanoparticles to purity. Soft Matter, 2019, 15, 7787-7794.	1.2	1
51	Charge transfer induced ferromagnetism and anomalous temperature increment of coercivity in ultrathin Î±-Fe ₂ O ₃ decorated graphene 2D nanostructures. Journal of Applied Physics, 2019, 125, .	1.1	9
52	Homonuclear B ₂ /B ₃ doped carbon allotropes as a universal gas sensor: Possibility of CO oxidation and CO ₂ hydrogenation. Carbon, 2019, 143, 38-50.	5.4	13
53	Ring type and Î€ electron occupancy decides the Li-ion storage properties of Phagraphene: An example of sp ² hybridized carbon structure. Carbon, 2018, 129, 775-784.	5.4	26
54	Structural and Electronic Descriptors of Catalytic Activity of Grapheneâ€™Based Materials: Firstâ€™Principles Theoretical Analysis. Small, 2018, 14, 1703609.	5.2	64

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55	Chemical modulation of valance band in delafossite structured CuFeO ₂ thin film and its photoresponse. <i>Materials Research Express</i> , 2018, 5, 015909.	0.8	11
56	Designing of stable and highly efficient ordered Pt ₂ CoNi ternary alloy electrocatalyst: The origin of dioxygen reduction activity. <i>Nano Energy</i> , 2018, 43, 219-227.	8.2	49
57	Role of Gd-doping in conduction mechanism of BFO-PZO nanocrystalline composites: Experimental and first-principles studies. <i>Journal of Alloys and Compounds</i> , 2018, 768, 198-213.	2.8	18
58	Induced ferromagnetism and metal-insulator transition due to a charge transfer effect in silver nanoparticle decorated MoS_2 . <i>Physical Review B</i> , 2018, 98, .		10
59	Resonant energy transfer in a van der Waals stacked MoS ₂ functionalized graphene quantum dot composite with <i>ab initio</i> validation. <i>Nanoscale</i> , 2018, 10, 16822-16829.	2.8	10
60	Origin of spin polarization in an edge boron doped zigzag graphene nanoribbon: a potential spin filter. <i>Nanotechnology</i> , 2018, 29, 345203.	1.3	7
61	Electron doped C ₂ N monolayer as efficient noble metal-free catalysts for CO oxidation. <i>Applied Surface Science</i> , 2017, 418, 92-98.	3.1	24
62	Antiferro-ferromagnetic transition in ultrathin Ni(OH) ₂ layer grown on graphene surface and observation of interlayer exchange coupling in Ni(OH) ₂ /graphene/Ni(OH) ₂ nanostructures. <i>Applied Physics Letters</i> , 2017, 110, .	1.5	16
63	Schottky diode behaviour with excellent photoresponse in NiO/FTO heterostructure. <i>Applied Surface Science</i> , 2017, 418, 328-334.	3.1	68
64	Asian consortium on computational materials science theme meeting on "first principles analysis & experiment: Role in energy research" 24 september 2016, SRM University, Kattankulathur, Chennai, India (ACCMS-TM 2016). <i>Applied Surface Science</i> , 2017, 418, 1.	3.1	1
65	First-principles identification of site dependent activity of graphene based electrocatalyst. <i>Molecular Catalysis</i> , 2017, 432, 242-249.	1.0	6
66	Role of oxygen functionality on the band structure evolution and conductance of reduced graphene oxide. <i>Chemical Physics Letters</i> , 2017, 677, 80-86.	1.2	15
67	Flexible diode of polyaniline/ITO heterojunction on PET substrate. <i>Applied Surface Science</i> , 2017, 418, 264-269.	3.1	49
68	Effect of Mg substitution in delafossite structured CuFeO ₂ thin film deposited on FTO coated glass substrate and its diode characteristics. <i>Thin Solid Films</i> , 2017, 642, 316-323.	0.8	22
69	Ag nanoparticle decorated molybdenum oxide structures: growth, characterization, DFT studies and their application to enhanced field emission. <i>Nanotechnology</i> , 2017, 28, 415602.	1.3	14
70	Screening based approach and dehydrogenation kinetics for MgH ₂ : Guide to find suitable dopant using first-principles approach. <i>Scientific Reports</i> , 2017, 7, 15550.	1.6	26
71	Exploring the catalytic activity of pristine T6[100] surface for oxygen reduction reaction: A first-principles study. <i>Applied Surface Science</i> , 2017, 418, 56-63.	3.1	5
72	Si doped T6 carbon structure as an anode material for Li-ion batteries: An <i>ab initio</i> study. <i>Scientific Reports</i> , 2016, 6, 37822.	1.6	6

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73	Spillover of hydrogen on SiC-ML surface: Doping effect and bond exchange mechanism. International Journal of Hydrogen Energy, 2016, 41, 3928-3939.	3.8	9
74	Mixed phase delafossite structured p type CuFeO ₂ /CuO thin film on FTO coated glass and its Schottky diode characteristics. Microelectronic Engineering, 2016, 162, 23-26.	1.1	31
75	Tuning the work function of randomly oriented ZnO nanostructures by capping with faceted Au nanostructure and oxygen defects: enhanced field emission experiments and DFT studies. Nanotechnology, 2016, 27, 125701.	1.3	36
76	Effect of multiple defects and substituted impurities on the band structure of graphene: a DFT study. Journal of Materials Science: Materials in Electronics, 2016, 27, 12669-12679.	1.1	13
77	CO Oxidation Prefers the Eley- Rideal or Langmuir- Hinshelwood Pathway: Monolayer vs Thin Film of SiC. ACS Applied Materials & Interfaces, 2016, 8, 5290-5299.	4.0	44
78	Colossal magnetoresistance in amino-functionalized graphene quantum dots at room temperature: manifestation of weak anti-localization and doorway to spintronics. Nanoscale, 2016, 8, 8245-8254.	2.8	6
79	Effect of surface doping on the band structure of graphene: a DFT study. Journal of Materials Science: Materials in Electronics, 2016, 27, 2728-2740.	1.1	16
80	Activation of CO and CO ₂ on homonuclear boron bonds of fullerene-like BN cages: first principles study. Scientific Reports, 2015, 5, 17460.	1.6	36
81	First principles design of divacancy defected graphene nanoribbon based rectifying and negative differential resistance device. AIP Advances, 2015, 5, .	0.6	23
82	Hydrogen spillover on DV (555-777) graphene - vanadium cluster system: First principles study. AIP Conference Proceedings, 2015, . .	0.3	2
83	First principle identification of SiC monolayer as an efficient catalyst for CO oxidation. AIP Conference Proceedings, 2015, . .	0.3	0
84	In plane conducting channel at the interface of CdO- ZnO isotype thin film heterostructure. Journal of Alloys and Compounds, 2015, 632, 343-347.	2.8	24
85	An oxygen reduction catalytic process through superoxo adsorption states on n-type doped h-BN: A first-principles study. Current Applied Physics, 2015, 15, 727-732.	1.1	15
86	Facile synthesis of Ag nanowire- rGO composites and their promising field emission performance. RSC Advances, 2015, 5, 41887-41893.	1.7	34
87	Self-Size-Limiting Nanoscale Perforation of Graphene for Dense Heteroatom Doping. ACS Applied Materials & Interfaces, 2015, 7, 25898-25905.	4.0	24
88	Influence of enolate/epoxy configuration, doping and vacancy on the catalytic activity of graphene. RSC Advances, 2015, 5, 93215-93225.	1.7	20
89	Enhanced electron field emission from NiCo ₂ O ₄ nanosheet arrays. Materials Research Express, 2015, 2, 095011.	0.8	26
90	Efficient Field Emission from Vertically Aligned Cu ₂ O- ZnO (111) Nanostructure Influenced by Oxygen Vacancy. Advanced Functional Materials, 2015, 25, 947-956.	7.8	42

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91	Field emission properties of spinel ZnCo ₂ O ₄ microflowers. RSC Advances, 2015, 5, 5372-5378.	1.7	55
92	First principles guide to tune h-BN nanostructures as superior light-element-based hydrogen storage materials: role of the bond exchange spillover mechanism. Journal of Materials Chemistry A, 2015, 3, 304-313.	5.2	39
93	Magnetic, elastic and optical properties of zinc peroxide (ZnO ₂): First principles study. Journal of Alloys and Compounds, 2015, 620, 156-163.	2.8	11
94	Field emission properties of ZnO nanosheet arrays. Applied Physics Letters, 2014, 105, .	1.5	51
95	Amino-functionalized graphene quantum dots: origin of tunable heterogeneous photoluminescence. Nanoscale, 2014, 6, 3384.	2.8	237
96	<i>Ab Initio</i> Study of Thin Oxide/Metal Overlayers as an Inverse Catalytic System for Dioxygen Reduction and Enhanced CO Tolerance. ACS Catalysis, 2014, 4, 4074-4080.	5.5	42
97	A first-principles investigation of oxygen reduction reaction catalysis capabilities of As decorated defect graphene. Dalton Transactions, 2014, 43, 15038-15047.	1.6	5
98	Doped h-BN monolayer as efficient noble metal-free catalysts for CO oxidation: the role of dopant and water in activity and catalytic de-poisoning. Journal of Materials Chemistry A, 2014, 2, 12812-12820.	5.2	76
99	Rules of Boron/Nitrogen Doping in Defect Graphene Sheets: A First-Principles Investigation of Band-Gap Tuning and Oxygen Reduction Reaction Catalysis Capabilities. ChemPhysChem, 2014, 15, 2542-2549.	1.0	41
100	Optical and vibrational properties of hydrogenated BN-sheet: First principles study. Applied Surface Science, 2013, 284, 638-643.	3.1	6
101	Small Pd cluster adsorbed double vacancy defect graphene sheet for hydrogen storage: A first-principles study. International Journal of Hydrogen Energy, 2013, 38, 3041-3049.	3.8	83
102	Promotion of oxygen reduction by a bio-inspired tethered iron phthalocyanine carbon nanotube-based catalyst. Nature Communications, 2013, 4, 2076.	5.8	630
103	Site dependent metal adsorption on (3 Å × 3) h-BN monolayer: Stability, magnetic and optical properties. Computational Materials Science, 2012, 51, 165-171.	1.4	23
104	First-Principles Identification of Iodine Exchange Mechanism in Iodide Ionic Liquid. Journal of Physical Chemistry Letters, 2012, 3, 3065-3069.	2.1	27
105	Structural transformation from Mn ₃ O ₄ nanorods to nanoparticles and band gap tuning via Zn doping. Materials Research Bulletin, 2012, 47, 813-819.	2.7	52
106	SPECTROSCOPIC ELLIPSOMETRIC STUDIES ON THE OPTICAL PROPERTIES OF PHOSPHORUS DOPED NANOCRYSTALLINE NiO THIN FILMS. International Journal of Nanoscience, 2011, 10, 985-988.	0.4	3
107	Temperature-dependent ac conductivity and dielectric response of vanadium doped CaCu ₃ Ti ₄ O ₁₂ ceramic. Applied Physics A: Materials Science and Processing, 2011, 104, 1105-1111.	1.1	13
108	Palladium atoms and its dimers adsorbed on graphene: First-principles study. Physica B: Condensed Matter, 2011, 406, 368-373.	1.3	41

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109	QUANTUM SIZE EFFECT ON THE OPTICAL PROPERTIES OF RF MAGNETRON SPUTTERED NANOCRYSTALLINE CADMIUM OXIDE THIN FILMS. International Journal of Nanoscience, 2011, 10, 713-716.	0.4	4
110	Optical and electrical properties of p-type transparent conducting CuAlO ₂ thin film synthesized by reactive radio frequency magnetron sputtering technique. Indian Journal of Physics, 2010, 84, 1341-1346.	0.9	18
111	Study of field emission and dielectric properties of AlN films prepared by DC sputtering technique at different substrate temperatures. Indian Journal of Physics, 2010, 84, 1347-1354.	0.9	12
112	Band gap widening of nanocrystalline nickel oxide thin films via phosphorus doping. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 1377-1382.	1.3	47
113	Self filling of Ni nanoparticles in amorphous AlN nanotubes and its field emission property. Applied Surface Science, 2010, 256, 3988-3992.	3.1	21
114	Flexible cold cathode with ultralow threshold field designed through wet chemical route. Nanotechnology, 2010, 21, 505701.	1.3	27
115	Effect of vanadium doping on the dielectric and nonlinear current-voltage characteristics of CaCu ₃ Ti ₄ O ₁₂ ceramic. Journal of Alloys and Compounds, 2010, 506, 853-857.	2.8	35
116	First principles analysis on V ³⁺ doped aluminum nitride. Computational Materials Science, 2010, 49, 363-367.	1.4	9
117	A novel route for the low temperature synthesis of p-type transparent semiconducting CuAlO ₂ . Materials Letters, 2009, 63, 394-396.	1.3	21
118	Enhanced field emission from Si doped nanocrystalline AlN thin films. Applied Surface Science, 2009, 255, 4536-4541.	3.1	16
119	Synthesis of cubic aluminum nitride by VLS technique using gold chloride as a catalyst and its optical and field emission properties. Journal of Alloys and Compounds, 2009, 475, 373-377.	2.8	16
120	Optical and dielectric properties of PVA capped nanocrystalline PbS thin films synthesized by chemical bath deposition. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 3121-3126.	1.3	89
121	Bandgap widening in highly conducting CdO thin film by Ti incorporation through radio frequency magnetron sputtering technique. Solid State Communications, 2008, 145, 33-37.	0.9	118
122	Improvement of electrical and thermoelectric properties of CdO thin film by aluminum doping. , 2007, , .		1
123	Highly efficient catalysts of ruthenium clusters on Fe ₃ O ₄ /MWCNTs for the hydrogen evolution reaction. New Journal of Chemistry, 0, , .	1.4	5