

Tanveer Hussain

List of Publications by Year in descending order

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104
papers

3,463
citations

101384

36
h-index

174990

52
g-index

105
all docs

105
docs citations

105
times ranked

2658
citing authors

#	ARTICLE	IF	CITATIONS
1	Sulfur encapsulation into yolk-shell Fe ₂ N@nitrogen doped carbon for ambient-temperature sodium-sulfur battery cathode. <i>Chemical Engineering Journal</i> , 2022, 429, 132389.	6.6	26
2	Two-dimensional Nitrogenated Holey Graphene (C ₂ N) monolayer based glucose sensor for diabetes mellitus. <i>Applied Surface Science</i> , 2022, 573, 151579.	3.1	20
3	Stabilizing Interface pH by Na ⁺ -Modified Graphdiyne for Dendrite-Free and High-Rate Aqueous Zn-Ion Batteries. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	24
4	Charge Storage Behaviour of $\text{La}^{\pm}\text{MoO}_3$ in Aqueous Electrolytes – Effect of Charge Density of Electrolyte Cations. <i>ChemElectroChem</i> , 2022, 9, .	1.7	5
5	Designing two-dimensional dodecagonal boron nitride. <i>CrystEngComm</i> , 2022, 24, 471-474.	1.3	7
6	Boron-Rich Boron Nitride Nanotubes as Highly Selective Adsorbents for Selected Diatomic Air Pollutants: A DFT Study. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	8
7	Modified KBBF-like Material for Energy Storage Applications: ZnNiBO ₃ (OH) with Enhanced Cycle Life. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 8025-8035.	4.0	20
8	High-capacity reversible hydrogen storage properties of metal-decorated nitrogenated holey graphenes. <i>International Journal of Hydrogen Energy</i> , 2022, 47, 10654-10664.	3.8	22
9	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. <i>ACS Applied Nano Materials</i> , 2022, 5, 2984-2993.	2.4	29
10	Elucidating Synergistic Mechanisms of Adsorption and Electrocatalysis of Polysulfides on Double-Transition Metal MXenes for Na-S Batteries. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 10298-10307.	4.0	18
11	Tuning the electronic, magnetic, and sensing properties of a single atom embedded microporous C ₃ N ₆ monolayer towards XO ₂ (X = C, N, S) gases. <i>New Journal of Chemistry</i> , 2022, 46, 13752-13765.	1.4	5
12	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.	1.4	21
13	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.	3.8	63
14	Integration of CuO nanosheets to Zn-Ni-Co oxide nanowire arrays for energy storage applications. <i>Chemical Engineering Journal</i> , 2021, 413, 127570.	6.6	70
15	Scavenging properties of yttrium nitride monolayer towards toxic sulfur gases. <i>Applied Surface Science</i> , 2021, 537, 147711.	3.1	8
16	Mechanistic Understanding of the Interactions and Pseudocapacitance of Multi-Electron Redox Organic Molecules Sandwiched between MXene Layers. <i>Advanced Electronic Materials</i> , 2021, 7, 2001202.	2.6	10
17	Two-dimensional Janus monolayers of MoSSe as promising sensor towards selected adulterants compounds. <i>Applied Surface Science</i> , 2021, 542, 148590.	3.1	29
18	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.	2.5	10

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19	Antimonene Allotropes $\hat{1}$ - and $\hat{2}$ -Phases as Promising Anchoring Materials for Lithium-Sulfur Batteries. <i>Energy & Fuels</i> , 2021, 35, 9001-9009.	2.5	15
20	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.	2.4	9
21	Rationalized atomic/clusters dispersion of Fe/Se/Al on interconnected N-doped carbon nanofibers for fast sodiation. <i>Chemical Engineering Journal</i> , 2021, 411, 128420.	6.6	5
22	A manganese hexacyanoferrate framework with enlarged ion tunnels and two-species redox reaction for aqueous Al-ion batteries. <i>Nano Energy</i> , 2021, 84, 105945.	8.2	54
23	Enhancing energy storage efficiency of lithiated carbon nitride (C ₇ N ₆) monolayers under co-adsorption of H ₂ and CH ₄ . <i>International Journal of Hydrogen Energy</i> , 2021, 46, 19988-19997.	3.8	19
24	Substituted 2D Janus WSSe monolayers as efficient nanosensor toward toxic gases. <i>Journal of Applied Physics</i> , 2021, 130, .	1.1	16
25	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.	2.5	3
26	Application of germanene monolayers as efficient anchoring material to immobilize lithium polysulfides in Li-S batteries. <i>Applied Surface Science</i> , 2021, 558, 149850.	3.1	8
27	The effect of Na addition on the first hydrogen absorption kinetics of cast hypoeutectic Mg-La alloys. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 27096-27106.	3.8	10
28	How to avoid dendrite formation in metal batteries: Innovative strategies for dendrite suppression. <i>Nano Energy</i> , 2021, 86, 106142.	8.2	116
29	Empowering hydrogen storage properties of haeckelite monolayers via metal atom functionalization. <i>Applied Surface Science</i> , 2021, 556, 149709.	3.1	20
30	Binder-free trimetallic phosphate nanosheets as an electrode: Theoretical and experimental investigation. <i>Journal of Power Sources</i> , 2021, 513, 230556.	4.0	45
31	Conversion of CO ₂ into Formic Acid on Transition Metal-Porphyrin-like Graphene: First Principles Calculations. <i>ACS Omega</i> , 2021, 6, 27045-27051.	1.6	3
32	Investigating CO ₂ storage properties of C ₂ N monolayer functionalized with small metal clusters. <i>Journal of CO₂ Utilization</i> , 2020, 35, 1-13.	3.3	20
33	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.	3.8	110
34	Influence of Sodium Iodide doped polypyrrole on green synthesized aluminum doped ZnO for the enhanced charge separation at the interface. <i>Optical Materials</i> , 2020, 99, 109568.	1.7	6
35	Ammonia gas adsorption study on graphene oxide based sensing device under different humidity conditions. <i>Materials Chemistry and Physics</i> , 2020, 242, 122485.	2.0	24
36	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.	5.4	29

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37	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.	1.5	5
38	Superior Anchoring of Sodium Polysulfides to the Polar C ₂ N 2D Material: A Potential Electrode Enhancer in Sodium-Sulfur Batteries. <i>Langmuir</i> , 2020, 36, 13104-13111.	1.6	27
39	Tuning Hydrogen Storage Properties of Carbonene Nanosheets through Selected Foreign Metal Functionalization. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16827-16837.	1.5	15
40	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.	4.0	53
41	Density Functional Theory Studies of Si ₂ BN Nanosheets as Anode Materials for Magnesium-Ion Batteries. <i>ACS Applied Nano Materials</i> , 2020, 3, 9055-9063.	2.4	40
42	Elucidating hydrogen storage properties of two-dimensional siligraphene (SiC ₈) monolayers upon selected metal decoration. <i>Sustainable Energy and Fuels</i> , 2020, 4, 5578-5587.	2.5	22
43	Efficient Sensing Properties of Aluminum Nitride Nanosheets toward Toxic Pollutants under Gated Electric Field. <i>ACS Applied Electronic Materials</i> , 2020, 2, 1645-1652.	2.0	15
44	Potassium Poly(Heptazine Imide): Transition Metal-Free Solid-State Triplet Sensitizer in Cascade Energy Transfer and [3+2] Cycloadditions. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15061-15068.	7.2	91
45	Transition of wide-band gap semiconductor h-BN(BN)/P heterostructure via single-atom-embedding. <i>Journal of Materials Chemistry C</i> , 2020, 8, 9755-9762.	2.7	7
46	Sensing of volatile organic compounds on two-dimensional nitrogenated holey graphene, graphdiyne, and their heterostructure. <i>Carbon</i> , 2020, 163, 213-223.	5.4	77
47	The adsorption and migration behavior of divalent metals (Mg, Ca, and Zn) on pristine and defective graphene. <i>Carbon</i> , 2020, 163, 276-287.	5.4	36
48	Physisorption and Chemisorption of SF ₆ by Transition Metal-Porphyrin Structure Embedded on Graphene Surface with Different Hapticities. <i>Journal of the Korean Physical Society</i> , 2020, 76, 1001-1004.	0.3	1
49	Capacity enhancement of polythiated functionalized boron nitride nanotubes: an efficient hydrogen storage medium. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15675-15682.	1.3	18
50	Highly sensitive and selective sensing properties of modified green phosphorene monolayers towards SF ₆ decomposition gases. <i>Applied Surface Science</i> , 2020, 512, 145641.	3.1	28
51	Superior sensitivity of metal functionalized boron carbide (BC ₃) monolayer towards carbonaceous pollutants. <i>Applied Surface Science</i> , 2020, 512, 145637.	3.1	15
52	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.	1.5	28
53	Moiré patterns arising from bilayer graphone/graphene superlattice. <i>Nano Research</i> , 2020, 13, 1060-1064.	5.8	11
54	Sensitivity enhancement of stanene towards toxic SO ₂ and H ₂ S. <i>Applied Surface Science</i> , 2019, 495, 143622.	3.1	17

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55	Encapsulating Trogtalite CoSe_2 Nanobuds into BCN Nanotubes as High Storage Capacity Sodium Ion Battery Anodes. <i>Advanced Energy Materials</i> , 2019, 9, 1901778.	10.2	131
56	Three-Dimensional Silicon Carbide from Siligraphene as a High Capacity Lithium Ion Battery Anode Material. <i>Journal of Physical Chemistry C</i> , 2019, 123, 27295-27304.	1.5	26
57	Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe_2 and Tj ETQq1)	1.0784314	101
58	Computational Study on the Adsorption of Sodium and Calcium on Edge-Functionalized Graphene Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14895-14908.	1.5	23
59	Reversible hydrogen storage properties of defect-engineered C_4N nanosheets under ambient conditions.	5.4	69
60	Blue phosphorene monolayers as potential nano sensors for volatile organic compounds under point defects. <i>Applied Surface Science</i> , 2019, 486, 52-57.	3.1	87
61	Enhancement in hydrogen storage capacities of light metal functionalized Boron Graphdiyne nanosheets. <i>Carbon</i> , 2019, 147, 199-205.	5.4	100
62	Theoretical realization of two-dimensional $\text{M}_3(\text{C}_6\text{X}_6)_2$ ($\text{M} = \text{Co, Cr, Cu, Fe, Mn, Ni, Pd, Rh}$ and $\text{X} = \text{O, S}$).	0.0	37
63	N-, B-, P-, Al-, As-, and Ga-graphdiyne/graphyne lattices: first-principles investigation of mechanical, optical and electronic properties. <i>Journal of Materials Chemistry C</i> , 2019, 7, 3025-3036.	2.7	41
64	Metal functionalized inorganic nano-sheets as promising materials for clean energy storage. <i>Applied Surface Science</i> , 2019, 471, 887-892.	3.1	39
65	Tailoring the capability of carbon nitride (C_3N) nanosheets toward hydrogen storage upon light transition metal decoration. <i>Nanotechnology</i> , 2019, 30, 075404.	1.3	40
66	Hydrogenated defective graphene as an anode material for sodium and calcium ion batteries: A density functional theory study. <i>Carbon</i> , 2018, 136, 73-84.	5.4	52
67	Metallized siligraphene nanosheets (SiC_7) as high capacity hydrogen storage materials. <i>Nano Research</i> , 2018, 11, 3802-3813.	5.8	48
68	Defected and Functionalized Germanene-based Nanosensors under Sulfur Comprising Gas Exposure. <i>ACS Sensors</i> , 2018, 3, 867-874.	4.0	53
69	Adsorption characteristics of DNA nucleobases, aromatic amino acids and heterocyclic molecules on silicene and germanene monolayers. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2713-2720.	4.0	56
70	Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional Si_2BN . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21716-21723.	1.3	30
71	Theoretical Investigation of Metallic Nanolayers For Charge-Storage Applications. <i>ACS Applied Energy Materials</i> , 2018, 1, 3428-3433.	2.5	19
72	Efficient Adsorption Characteristics of Pristine and Silver-Doped Graphene Oxide Towards Contaminants: A Potential Membrane Material for Water Purification?. <i>ChemPhysChem</i> , 2018, 19, 2250-2257.	1.0	14

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73	Hexagonal Boron Nitride (h-BN) Sheets Decorated with OLi, ONa, and Li ₂ F Molecules for Enhanced Energy Storage. ChemPhysChem, 2017, 18, 513-518.	1.0	41
74	Sodium-intercalated bulk graphdiyne as an anode material for rechargeable batteries. Journal of Power Sources, 2017, 343, 354-363.	4.0	66
75	Improving Sensing of Sulfur-Containing Gas Molecules with ZnO Monolayers by Implanting Dopants and Defects. Journal of Physical Chemistry C, 2017, 121, 24365-24375.	1.5	35
76	Improved sensing characteristics of methane over ZnO nano sheets upon implanting defects and foreign atoms substitution. Nanotechnology, 2017, 28, 415502.	1.3	17
77	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. Journal of Physical Chemistry C, 2017, 121, 14393-14400.	1.5	65
78	Sensing Characteristics of Phosphorene Monolayers toward PH ₃ and AsH ₃ Gases upon the Introduction of Vacancy Defects. Journal of Physical Chemistry C, 2016, 120, 20428-20436.	1.5	71
79	Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. Journal of Physical Chemistry C, 2016, 120, 25256-25262.	1.5	81
80	Computational Evaluation of Lithium-Functionalized Carbon Nitride (g-C ₆ N ₈) Monolayer as an Efficient Hydrogen Storage Material. Journal of Physical Chemistry C, 2016, 120, 25180-25188.	1.5	76
81	Reversible Hydrogen Uptake by BN and BC ₃ Monolayers Functionalized with Small Fe Clusters: A Route to Effective Energy Storage. Journal of Physical Chemistry A, 2016, 120, 2009-2013.	1.1	39
82	Designing Square Two-Dimensional Gold and Platinum. Crystal Growth and Design, 2016, 16, 1746-1750.	1.4	15
83	Sensing Characteristics of a Graphene-like Boron Carbide Monolayer towards Selected Toxic Gases. ChemPhysChem, 2015, 16, 3511-3517.	1.0	25
84	Improvement in Hydrogen Desorption from \hat{I}^2 and \hat{I}^3 MgH ₂ upon Transition-Metal Doping. ChemPhysChem, 2015, 16, 2557-2561.	1.0	22
85	Improvement in Hydrogen Desorption from \hat{I}^2 - and \hat{I}^3 -MgH ₂ upon Transition-Metal Doping. ChemPhysChem, 2015, 16, 2481-2481.	1.0	0
86	Complementing the adsorption energies of CO ₂ , H ₂ S and NO ₂ to h-BN sheets by doping with carbon. Europhysics Letters, 2015, 109, 57008.	0.7	24
87	BC ₃ Sheet Functionalized with Lithium-Rich Species Emerging as a Reversible Hydrogen Storage Material. ChemPhysChem, 2015, 16, 634-639.	1.0	9
88	Enhancement of energy storage capacity of Mg functionalized silicene and silicane under external strain. Applied Physics Letters, 2014, 105, .	1.5	29
89	Sensing propensity of a defected graphane sheet towards CO, H ₂ O and NO ₂ . Nanotechnology, 2014, 25, 325501.	1.3	53
90	Hole induced Jahn Teller distortion ensuing ferromagnetism in Mn ²⁺ MgO: bulk, surface and one dimensional structures. Journal of Physics Condensed Matter, 2014, 26, 265801.	0.7	3

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91	Improvement in the desorption of H ₂ from the MgH ₂ (110) surface by means of doping and mechanical strain. Computational Materials Science, 2014, 86, 165-169.	1.4	9
92	Functionalization of hydrogenated graphene by polyolithiated species for efficient hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 2560-2566.	3.8	40
93	Enriching physisorption of H ₂ and NH ₃ gases on a graphene sheet by doping with Li adatoms. Physical Chemistry Chemical Physics, 2014, 16, 8100-8105.	1.3	53
94	Metal-Functionalized Silicene for Efficient Hydrogen Storage. ChemPhysChem, 2013, 14, 3463-3466.	1.0	45
95	Hydrogen storage in polyolithiated BC ₃ monolayer sheet. Solid State Communications, 2013, 170, 39-43.	0.9	29
96	Functionalization of hydrogenated silicene with alkali and alkaline earth metals for efficient hydrogen storage. Physical Chemistry Chemical Physics, 2013, 15, 18900.	1.3	45
97	Strain and doping effects on the energetics of hydrogen desorption from the MgH ₂ (001) surface. Europhysics Letters, 2013, 101, 27006.	0.7	13
98	Improvement in the hydrogen desorption from MgH ₂ upon transition metals doping: A hybrid density functional calculations. AIP Advances, 2013, 3, .	0.6	11
99	Hexagonal Boron Nitride Sheet Decorated by Polyolithiated Species for Efficient and Reversible Hydrogen Storage. Science of Advanced Materials, 2013, 5, 1960-1966.	0.1	5
100	Polyolithiated (OLi ₂) functionalized graphane as a potential hydrogen storage material. Applied Physics Letters, 2012, 101, 243902.	1.5	11
101	Strain induced lithium functionalized graphane as a high capacity hydrogen storage material. Applied Physics Letters, 2012, 101, .	1.5	55
102	Structural, electronic and thermodynamic properties of Al- and Si-doped $\hat{1}^{\pm}$, $\hat{1}^3$, and $\hat{1}^2$ -MgH ₂ : Density functional and hybrid density functional calculations. International Journal of Hydrogen Energy, 2012, 37, 9112-9122.	3.8	27
103	Functionalized Boranes for Hydrogen Storage. ChemPhysChem, 2012, 13, 300-304.	1.0	22
104	Ab initio study of lithium-doped graphane for hydrogen storage. Europhysics Letters, 2011, 96, 27013.	0.7	48