

Biswarup Pathak

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190
papers

4,064
citations

35
h-index

55
g-index

212
ext. papers

5,036
ext. citations

5.1
avg, IF

6.25
L-index

#	Paper	IF	Citations
190	High-energy-density dual-ion battery for stationary storage of electricity using concentrated potassium fluorosulfonylimide. <i>Nature Communications</i> , 2018 , 9, 4469	17.4	140
189	Transverse conductance of DNA nucleotides in a graphene nanogap from first principles. <i>Nano Letters</i> , 2011 , 11, 1941-5	11.5	138
188	Guest-Induced Ultrasensitive Detection of Multiple Toxic Organics and Fe Ions in a Strategically Designed and Regenerative Smart Fluorescent Metal-Organic Framework. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 9042-9053	9.5	117
187	The staging mechanism of AlCl ₃ intercalation in a graphite electrode for an aluminium-ion battery. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 7980-7989	3.6	104
186	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. <i>Journal of Catalysis</i> , 2013 , 299, 204-209	7.3	101
185	Graphene-like Carbon Nitride Monolayer: A Potential Anode Material for Na- and K-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 2481-2489	3.8	99
184	Hexagonal Planar CdS Monolayer Sheet for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 7052-7060	3.8	96
183	Room-temperature chemoselective reduction of nitro groups using non-noble metal nanocatalysts in water. <i>Inorganic Chemistry</i> , 2014 , 53, 2904-9	5.1	92
182	B: Highly Sensitive and Selective Gas Sensor. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24827-24836	3.8	87
181	Calcium doped graphane as a hydrogen storage material. <i>Applied Physics Letters</i> , 2012 , 100, 183902	3.4	82
180	Direct vs. indirect pathway for nitrobenzene reduction reaction on a Ni catalyst surface: a density functional study. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 26365-74	3.6	81
179	Theoretical Study of Electronic Transport through DNA Nucleotides in a Double-Functionalized Graphene Nanogap. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 15421-15428	3.8	74
178	Cardanol benzoxazines [Interplay of oxazine functionality (mono to tetra) and properties. <i>RSC Advances</i> , 2015 , 5, 78071-78080	3.7	67
177	Anaerobic photocleavage of DNA in red light by dicopper(II) complexes of 3,3Pdithiodipropionic acid. <i>Inorganic Chemistry</i> , 2009 , 48, 339-49	5.1	67
176	Anion-Doped NaTaO ₃ for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 22518-22524	3.2	63
175	Borane derivatives: a new class of super- and hyperhalogens. <i>ChemPhysChem</i> , 2011 , 12, 2423-8	3.2	63
174	New insights into the visible-light-induced DNA cleavage activity of dipyridoquinoxaline complexes of bivalent 3d-metal ions. <i>Inorganic Chemistry</i> , 2007 , 46, 11122-32	5.1	62

173	Hybrid density functional study on SrTiO ₃ for visible light photocatalysis. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 11611-11617	6.7	61
172	Recent Advances in Graphene-like 2D Materials for Spintronics Applications. <i>Chemistry of Materials</i> , 2019 , 31, 8260-8285	9.6	60
171	Antibiotic-triggered reversible luminescence switching in amine-grafted mixed-linker MOF: exceptional turn-on and ultrafast nanomolar detection of sulfadiazine and adenosine monophosphate with molecular keypad lock functionality. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 19471-19484	13	56
170	Access to highly active NiPd bimetallic nanoparticle catalysts for C-C coupling reactions. <i>Catalysis Science and Technology</i> , 2016 , 6, 5567-5579	5.5	54
169	Electronic Structure, Optical Properties, and Photocatalytic Activities of LaFeO ₃ /NaTaO ₃ Solid Solution. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 22767-22773	3.8	52
168	Band gap engineering in huge-gap semiconductor SrZrO ₃ for visible-light photocatalysis. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 2042-2048	6.7	51
167	Band gap engineering in BiNbO ₄ for visible-light photocatalysis. <i>Applied Physics Letters</i> , 2012 , 100, 182102	4	49
166	Recent advancements in Pt-nanostructure-based electrocatalysts for the oxygen reduction reaction. <i>Catalysis Science and Technology</i> , 2019 , 9, 4835-4863	5.5	47
165	Mo- and N-doped BiNbO ₄ for photocatalysis applications. <i>Applied Physics Letters</i> , 2011 , 99, 051909	3.4	46
164	Ab initio study of lithium-doped graphane for hydrogen storage. <i>Europhysics Letters</i> , 2011 , 96, 27013	1.6	44
163	Transition-metal embedded carbon nitride monolayers: high-temperature ferromagnetism and half-metallicity. <i>Nanoscale</i> , 2016 , 8, 14117-26	7.7	42
162	First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2016 , 41, 14437-14446	6.7	42
161	Band gap opening in stanene induced by patterned B-N doping. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 3660-3669	3.6	41
160	Targeted water soluble copper-tetrazolate complexes: interactions with biomolecules and catecholase like activities. <i>Dalton Transactions</i> , 2015 , 44, 20154-67	4.3	41
159	Layered Perovskite Sr ₂ Ta ₂ O ₇ for Visible Light Photocatalysis: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5043-5050	3.8	41
158	Anion-Anion Mediated Coupling in Layered Perovskite La ₂ Ti ₂ O ₇ for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 13845-13852	3.8	39
157	Thermochemical and electrochemical CO ₂ reduction on octahedral Cu nanocluster: Role of solvent towards product selectivity. <i>Journal of Catalysis</i> , 2017 , 349, 118-127	7.3	37
156	Stanene based gas sensors: effect of spin-orbit coupling. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 31325-31334	3.6	37

155	Catalytic Hydrogenation of CO ₂ by Manganese Complexes: Role of π -Acceptor Ligands. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 16478-16488	3.8	34
154	Semiconducting allotrope of graphene. <i>Nanotechnology</i> , 2012 , 23, 385704	3.4	34
153	N-Heterocyclic Carbene-Based Mn Electrocatalyst for Two-Electron CO ₂ Reduction over Proton Reduction. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 8821-8831	3.8	34
152	Double-functionalized nanopore-embedded gold electrodes for rapid DNA sequencing. <i>Applied Physics Letters</i> , 2012 , 100, 023701	3.4	32
151	Bond length and bond multiplicity: sigma-bond prevents short pi-bonds. <i>Chemical Communications</i> , 2006 , 2164-6	5.8	32
150	Chemical Detoxification of Organomercurials. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 9323-9326	6.4	31
149	Coordination polymer hydrogels through Ag(I)-mediated spontaneous self-assembly of unsubstituted nucleobases and their antimicrobial activity. <i>RSC Advances</i> , 2016 , 6, 62968-62973	3.7	28
148	Single-layered platinum nanocage: a highly selective and efficient catalyst for fuel cells. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 12756-12767	13	28
147	Excellent Catalytic Effects of Graphene Nanofibers on Hydrogen Release of Sodium alanate. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 10861-10866	3.8	28
146	Hexagonal BC ₃ Electrode for a High-Voltage Al-Ion Battery. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 9748-9756	3.8	27
145	Fe doped LaGaO ₃ : good white light emitters. <i>RSC Advances</i> , 2016 , 6, 100230-100238	3.7	27
144	Computational Screening for ORR Activity of 3d Transition Metal Based M@Pt Core-Shell Clusters. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 3634-3644	3.8	27
143	Graphene/hBN Heterostructures as High-Capacity Cathodes with High Voltage for Next-Generation Aluminum Batteries. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 3959-3967	3.8	26
142	Metal-free half-metallicity in a high energy phase C-doped gh-C ₃ N ₄ system: a high Curie temperature planar system. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 11530-11539	7.1	26
141	Stereoselective synthesis of highly functionalized tetrahydrocarbazoles through a domino Michael-Henry reaction: an easy access to four contiguous chiral centers. <i>RSC Advances</i> , 2013 , 3, 10644	3.7	26
140	Screened hybrid density functional study on Sr ₂ Nb ₂ O ₇ for visible light photocatalysis. <i>Applied Physics Letters</i> , 2012 , 100, 181903	3.4	26
139	Pt ₃ Ti (Ti ₁₉ @Pt ₆₀)-Based Cuboctahedral Core-Shell Nanocluster Favors a Direct over Indirect Oxygen Reduction Reaction. <i>ACS Energy Letters</i> , 2016 , 1, 797-805	20.1	26
138	A free-standing platinum monolayer as an efficient and selective catalyst for the oxygen reduction reaction. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 5303-5313	13	25

137	Electronic Transport through DNA Nucleotides in Atomically Thin Phosphorene Electrodes for Rapid DNA Sequencing. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 219-225	9.5	25
136	Aliphatic MnBNP complexes for the CO ₂ hydrogenation reaction: a base free mechanism. <i>Catalysis Science and Technology</i> , 2017 , 7, 3234-3242	5.5	23
135	Lewis Acid-Base Adducts for Improving the Selectivity and Sensitivity of Graphene Based Gas Sensors. <i>ACS Sensors</i> , 2016 , 1, 451-459	9.2	23
134	Functionalization of graphane with alkali and alkaline-earth metals: An insulator-to-metallic transition. <i>Europhysics Letters</i> , 2012 , 99, 47004	1.6	23
133	Hole mediated coupling in Sr ₂ Nb ₂ O ₇ for visible light photocatalysis. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 4891-7	3.6	23
132	Tandem Si-C and C-H activation for decamethylhafnocene and bis(trimethylsilyl)acetylene. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 6907-10	16.4	23
131	Reversal of stability on metalation of pentagonal-bipyramidal (1-MB6H7(2-) 1-M-2-CB5H7(1-) and 1-M-2,4-C2B4H7) and Icosahedral (1-MB11H12(2-) 1-M-2-CB10H12(1-) and 1-M-2,4-C2B9H12) boranes (M = Al, Ga, In, and Tl): energetics of condensation and relationship to binuclear metallocenes. <i>Journal of the American Chemical Society</i> , 2006 , 128, 10915-22	16.4	23
130	Protection of Endogenous Thiols against Methylmercury with Benzimidazole-Based Thione by Unusual Ligand-Exchange Reactions. <i>Chemistry - A European Journal</i> , 2017 , 23, 5696-5707	4.8	21
129	Individual Identification of DNA Nucleobases on Atomically Thin Black Phosphorene Nanoribbons: van der Waals Corrected Density Functional Theory Calculations. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 22377-22383	3.8	21
128	TM@C ₃ N ₃ monolayers: high-temperature ferromagnetism and high anisotropy. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 8253-8262	7.1	20
127	Electron-rich graphite-like electrode: stability vs. voltage for Al batteries. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 10776-10786	13	20
126	Theoretical insights into CO ₂ hydrogenation to methanol by a MnBNP complex. <i>Catalysis Science and Technology</i> , 2019 , 9, 1867-1878	5.5	19
125	Cationic-anionic mediated charge compensation on La ₂ Ti ₂ O ₇ for visible light photocatalysis. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 17150-7	3.6	19
124	Cuboctahedral vs. octahedral platinum nanoclusters: insights into the shape-dependent catalytic activity for fuel cell applications. <i>Catalysis Science and Technology</i> , 2016 , 6, 7913-7923	5.5	19
123	High Curie temperature and half-metallicity in an atomically thin main group-based boron phosphide system: long range ferromagnetism. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22877-22889	3.6	18
122	Functionalized boranes for hydrogen storage. <i>ChemPhysChem</i> , 2012 , 13, 300-4	3.2	18
121	Chemical Detoxification of Organomercurials. <i>Angewandte Chemie</i> , 2015 , 127, 9455-9459	3.6	17
120	Dual-functionalization actuated trimodal attribute in an ultra-robust MOF: exceptionally selective capture and effectual fixation of CO ₂ with fast-responsive, nanomolar detection of assorted organo-contaminants in water. <i>Materials Chemistry Frontiers</i> , 2021 , 5, 979-994	7.8	17

119	A Computational Study of a Single-Walled Carbon-Nanotube-Based Ultrafast High-Capacity Aluminum Battery. <i>Chemistry - an Asian Journal</i> , 2017 , 12, 1944-1951	4.5	16
118	Troponate/Aminotroponate Ruthenium-Arene Complexes: Synthesis, Structure, and Ligand-Tuned Mechanistic Pathway for Direct C-H Bond Arylation with Aryl Chlorides in Water. <i>Inorganic Chemistry</i> , 2016 , 55, 6739-49	5.1	16
117	Catalytic Hydrogenation of CO ₂ by Fe Complexes Containing Pendant Amines: Role of Water and Base. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26652-26662	3.8	15
116	Quaternary Heusler alloy: An ideal platform to realize triple point fermions. <i>Physical Review B</i> , 2019 , 99,	3.3	14
115	A cuboctahedral platinum (Pt ₇₉) nanocluster enclosed by well defined facets favours di-sigma adsorption and improves the reaction kinetics for methanol fuel cells. <i>Nanoscale</i> , 2015 , 7, 13438-51	7.7	14
114	Metal-decorated graphene oxide for ammonia adsorption. <i>Europhysics Letters</i> , 2013 , 103, 28007	1.6	14
113	Water adsorption on ZnO(101 0): The role of intrinsic defects. <i>Europhysics Letters</i> , 2012 , 97, 17014	1.6	14
112	Theoretical study of the reaction of B ₂ H ₁₆ with MeCN: closo/closo to closo/nido conversion. <i>Inorganic Chemistry</i> , 2008 , 47, 4375-82	5.1	14
111	An atomically thin ferromagnetic half-metallic pyrazine-fused Mn-porphyrin sheet: a slow spin relaxation system. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 9069-9077	7.1	14
110	Role of Dimensionality for Photocatalytic Water Splitting: CdS Nanotube versus Bulk Structure. <i>ChemPhysChem</i> , 2019 , 20, 383-391	3.2	14
109	Bimetallic core-based cuboctahedral core-shell nanoclusters for the formation of hydrogen peroxide (2e reduction) over water (4e reduction): role of core metals. <i>Nanoscale</i> , 2017 , 9, 9537-9547	7.7	13
108	Metal-ligand bifunctional based Mn-catalysts for CO ₂ hydrogenation reaction. <i>Molecular Catalysis</i> , 2019 , 468, 109-116	3.3	13
107	Size Evolution Dynamics of Gold Nanoclusters at an Atom-Precision Level: Ligand Exchange, Growth Mechanism, Electrochemical, and Photophysical Properties. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 1781-1788	6.4	13
106	Octahedral Ni-nanocluster (Ni ₈₅) for Efficient and Selective Reduction of Nitric Oxide (NO) to Nitrogen (N ₂). <i>Scientific Reports</i> , 2016 , 6, 25590	4.9	13
105	Limiting nuclearity in formation of polynuclear metal complexes through [2 + 3] cycloaddition: synthesis and magnetic properties of tri- and pentanuclear metal complexes. <i>Dalton Transactions</i> , 2014 , 43, 8083-93	4.3	13
104	Ferromagnetism in magnesium chloride monolayer with an unusually large spin-up gap. <i>Nanoscale</i> , 2018 , 10, 22280-22292	7.7	13
103	High-Performance Water Harvester Framework for Triphasic and Synchronous Detection of Assorted Organotoxins with Site-Memory-Reliant Security Encryption via pH-Triggered Fluoroswitching. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 34012-34026	9.5	13
102	Computational Insights into the Working Mechanism of the LiPF ₆ /Graphite Dual-Ion Battery. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 23863-23871	3.8	12

101	A computational study on ligand assisted vs. ligand participation mechanisms for CO hydrogenation: importance of bifunctional ligand based catalysts. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 3932-3941	3.6	12
100	Semiconducting phase in borophene: role of defect and strain. <i>Journal Physics D: Applied Physics</i> , 2017 , 50, 405103	3	12
99	Kinetics behind a Strategy for Modulation of Sustainable Benzoxazines: Experimental Study and Its Theoretical Verification. <i>Macromolecular Chemistry and Physics</i> , 2016 , 217, 1342-1353	2.6	12
98	A computational study of electrocatalytic CO ₂ reduction by Mn(II) complexes: Role of bipyridine substituents. <i>Electrochimica Acta</i> , 2019 , 297, 606-612	6.7	12
97	Crystal-defect-induced facet-dependent electrocatalytic activity of 3D gold nanoflowers for the selective nanomolar detection of ascorbic acid. <i>Nanoscale</i> , 2018 , 10, 11091-11102	7.7	12
96	Room-Temperature Magneto-dielectric Effect in LaGaFeO ₃ ; Origin and Impact of Excess Oxygen. <i>Inorganic Chemistry</i> , 2017 , 56, 3809-3819	5.1	11
95	Structural and electrochemical aspects of tris(ferrocenyl/phenyl-ethynyl)phosphine ligated chalcogen bridged iron carbonyl clusters. <i>RSC Advances</i> , 2013 , 3, 26025	3.7	11
94	Ferromagnetism and Half-Metallicity in Atomically Thin Holey Nitrogenated Graphene Based Systems. <i>ChemPhysChem</i> , 2017 , 18, 2336-2346	3.2	11
93	Copper complexes with a flexible piperazinyl arm: nuclearity driven catecholase activity and interactions with biomolecules. <i>Journal of Coordination Chemistry</i> , 2016 , 69, 3619-3637	1.6	11
92	Density Functional Theory Study of Defect Induced Ferromagnetism and Half-Metallicity in CaI ₂ Based Monolayer for Spintronics Applications. <i>ACS Applied Nano Materials</i> , 2019 , 2, 6152-6161	5.6	10
91	Hexagonal CuCl Monolayer for Water Splitting: A DFT Study. <i>ACS Applied Nano Materials</i> , 2019 , 2, 4238-4246	4.4	10
90	Identification of Intermediate Au(SR) ₂ (SR) ₂ Cluster on Ligand-Induced Transformation of Au(SR) Nanocluster. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 4571-4576	6.4	10
89	Electronic Transport through DNA Nucleotides in BC ₃ Nanogap for Rapid DNA Sequencing. <i>ACS Applied Electronic Materials</i> , 2020 , 2, 1218-1225	4	10
88	Zn(II)-Nucleobase metal-organic nanofibers and nanoflowers: synthesis and photocatalytic application. <i>New Journal of Chemistry</i> , 2018 , 42, 17983-17990	3.6	10
87	Identifying suitable ionic liquid electrolytes for Al dual-ion batteries: role of electrochemical window, conductivity and voltage. <i>Materials Advances</i> , 2020 , 1, 1354-1363	3.3	9
86	Prospects of black phosphorus nanoribbon for explosive sensing: A computational approach. <i>Applied Surface Science</i> , 2020 , 529, 147094	6.7	9
85	Improvement in the hydrogen desorption from MgH ₂ upon transition metals doping: A hybrid density functional calculations. <i>AIP Advances</i> , 2013 , 3, 102117	1.5	9
84	Tandem-Aktivierung von Si-C- und C-H-Bindungen bei Decamethylhafnocen und Bis(trimethylsilyl)acetylen. <i>Angewandte Chemie</i> , 2007 , 119, 7031-7035	3.6	9

83	Machine Learning-Driven High-Throughput Screening of Alloy-Based Catalysts for Selective CO Hydrogenation to Methanol. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56151-56163	9.5	9
82	Functionalized carbon nanotube electrodes for controlled DNA sequencing. <i>Nanoscale Advances</i> , 2020 , 2, 4041-4050	5.1	9
81	Spin-Polarized Current in Ferromagnetic Half-Metallic Transition-Metal Iodide Nanowires. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 15717-15723	3.8	8
80	Enhanced Lewis acid-base adducts in doped stanene: Sensing and photocatalysis. <i>Applied Surface Science</i> , 2019 , 478, 946-958	6.7	8
79	Star shaped ferrocenyl substituted triphenylamines. <i>RSC Advances</i> , 2015 , 5, 71046-71051	3.7	8
78	Theoretical Insights into the Charge and Discharge Processes in Aluminum-Sulfur Batteries. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 11317-11324	3.8	8
77	Flexible proton-responsive ligand-based Mn(II) complexes for CO hydrogenation: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 12535-12542	3.6	8
76	Topologically protected hybrid states in graphene-stanene-graphene heterojunctions. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 1920-1925	7.1	8
75	Ferromagnetism and Half-Metallicity in a High-Band-Gap Hexagonal Boron Nitride System. <i>ChemPhysChem</i> , 2018 , 19, 153-161	3.2	8
74	Hexagonal Cu(111) Monolayers for Selective CO ₂ Hydrogenation to CH ₃ OH: Insights from Density Functional Theory. <i>ACS Applied Nano Materials</i> , 2019 , 2, 7686-7695	5.6	8
73	The effect of remote substitution on the formation of preferential isomers of cobalt(III)-tetrazolate complexes by microwave assisted cycloaddition. <i>Inorganic Chemistry Frontiers</i> , 2014 , 1, 599-610	6.8	8
72	The effect of remote substitution on formation of preferential geometrical isomer of cobalt(III)-tetrazolato complexes formed via [2 + 3] cycloaddition. <i>Inorganic Chemistry Communication</i> , 2013 , 34, 62-67	3.1	8
71	Theoretical investigations of the structure and bonding of several transition metal complexes to probe their carbon monoxide releasing properties. <i>International Journal of Quantum Chemistry</i> , 2009 , 109, 2263-2272	2.1	8
70	Emergence of Topological insulator and Nodal line semi-metal states in XXBi (X = Na, K, Rb, Cs; YP= Ca, Sr). <i>Scientific Reports</i> , 2019 , 9, 527	4.9	7
69	Computational Screening of Electrocatalytic Activity of Transition Metal-Doped CdS Nanotubes for Water Splitting. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 13419-13427	3.8	7
68	Catalytic upgrading of ethanol to n-butanol using an aliphatic Mn-BP complex: theoretical insights into reaction mechanisms and product selectivity. <i>Catalysis Science and Technology</i> , 2019 , 9, 2794-2805	5.5	7
67	Multilayered Platinum Nanotube for Oxygen Reduction in a Fuel Cell Cathode: Origin of Activity and Product Selectivity. <i>ACS Applied Energy Materials</i> , 2018 , 1, 3890-3899	6.1	7
66	Exploiting Le Chatelier's principle for a one-pot synthesis of nontoxic HHG NPs with the sharpest nanoscopic features suitable for tunable plasmon spectroscopy and high throughput SERS sensing. <i>Chemical Communications</i> , 2017 , 53, 10402-10405	5.8	7

65	Recent Trends in Electrode and Electrolyte Design for Aluminum Batteries. <i>ACS Omega</i> , 2021 , 6, 1043-1053	5.3	7
64	Energetic and structural analysis of N ₂ H ₄ BH ₃ inorganic solid and its modified material for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2013 , 38, 6718-6725	6.7	6
63	Strain-induced stabilization of Al functionalization in graphene oxide nanosheet for enhanced NH ₃ storage. <i>Applied Physics Letters</i> , 2013 , 102, 243905	3.4	6
62	Condensed two- and three-dimensional aromatic systems: a theoretical study on the relative stabilities of isomers of CB ₁₉ H ₁₆ ⁺ , B ₂₀ H ₁₅ Cl, and B ₂₀ H ₁₄ Cl ₂ and comparison to B ₁₂ H ₁₀ Cl ₂ ⁻ , C ₆ H ₄ Cl ₂ , C ₁₀ H ₇ Cl, and C ₁₀ H ₆ Cl ₂ . <i>Inorganic Chemistry</i> , 2005 , 44, 7184-8	5.1	6
61	Novel BCN-phosphorene bilayer: Dependence of carbon doping on band offsets for potential photovoltaic applications. <i>Applied Surface Science</i> , 2020 , 504, 144327	6.7	6
60	Defects Engineering on Ceria and C-C Coupling Reactions Using [Au(PPh) ₃] ⁺ Nanocluster: A Combined Experimental and Theoretical Study. <i>ACS Nano</i> , 2020 ,	16.7	6
59	Type-II Dirac states in full Heusler compounds XInPd ₂ (X = Ti, Zr, and Hf). <i>Physical Review B</i> , 2019 , 100,	3.3	6
58	Broken symmetry driven phase transitions from a topological semimetal to a gapped topological phase in SrAgAs. <i>Physical Review B</i> , 2019 , 99,	3.3	5
57	Extended topological line defects in graphene for individual identification of DNA nucleobases. <i>Materials Advances</i> , 2020 , 1, 2908-2916	3.3	5
56	Theoretical Insights into Solid Electrolyte Interphase Formation in an Al Anode Dual-Ion Battery. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7634-7643	3.8	5
55	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. <i>Nanoscale Advances</i> , 2020 , 2, 2410-2421	5.1	5
54	Effect on catecholase activity and interaction with biomolecules of metal complexes containing differently tuned 5-substituted ancillary tetrazolato ligands. <i>Polyhedron</i> , 2017 , 121, 155-171	2.7	5
53	Oxygen- and nitrogen-chemisorbed carbon nanostructures for Z-scheme photocatalysis applications. <i>Journal of Nanoparticle Research</i> , 2012 , 14, 1	2.3	5
52	Temperature-induced crystallinity and vibrational properties in samarium orthovanadate. <i>Physical Review B</i> , 2020 , 101,	3.3	5
51	Polycyclic Aromatic Hydrocarbons as Prospective Cathodes for Aluminum Organic Batteries. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 49-57	3.8	5
50	Identifying DNA Nucleotides via Transverse Electronic Transport in Atomically Thin Topologically Defected Graphene Electrodes.. <i>ACS Applied Bio Materials</i> , 2021 , 4, 1403-1412	4.1	5
49	Computational insights into selective CO ₂ hydrogenation to CH ₃ OH catalysed by ZnO based nanocages. <i>Materials Advances</i> , 2020 , 1, 2300-2309	3.3	5
48	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

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