Biswarup Pathak

List of Publications by Year in Descending Order

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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.

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	Graphene Nanoslit Device for Protein Sequencing: Ab Initio Quantum Transport Study. *ACS Applied Nano Materials*, **2022**, 5, 2715-2727	5.6	0
189	Size-Dependent Effects in Fullerene-Based Catalysts for Nonaqueous Li□Air Battery Applications. *ACS Applied Energy Materials*, **2022**, 5, 3380-3391	6.1	2
188	Strong anisotropy and band Gap engineering with mechanical strains in two-dimensional orthorhombic diboron dinitride (O-B2N2). *Applied Surface Science*, **2022**, 586, 152850	6.7	0
187	Solvent-Dependent Photophysical Properties of a Semiconducting One-Dimensional Silver Cluster-Assembled Material. *Inorganic Chemistry*, **2021**, 60, 18234-18241	5.1	1
186	Gold Deassembly: From Au(SPh-Bu) to Au(SPh-Bu) Nanocluster through Dynamic Surface Structure Reconstruction. *Journal of Physical Chemistry Letters*, **2021**, 12, 10987-10993	6.4	3
185	Density Functional Theory Calculations on Electrocatalytic CO2 Hydrogenation to C2-Based Products over Cu(100) Nanocubes. *ACS Applied Nano Materials*, **2021**, 4, 11907-11919	5.6	1
184	Machine Learning-Driven High-Throughput Screening of Alloy-Based Catalysts for Selective CO Hydrogenation to Methanol. *ACS Applied Materials & Interfaces*, **2021**, 13, 56151-56163	9.5	9
183	Polycyclic Aromatic Hydrocarbons as Prospective Cathodes for Aluminum Organic Batteries. *Journal of Physical Chemistry C*, **2021**, 125, 49-57	3.8	5
182	Identifying DNA Nucleotides via Transverse Electronic Transport in Atomically Thin Topologically Defected Graphene Electrodes.. *ACS Applied Bio Materials*, **2021**, 4, 1403-1412	4.1	5
181	Current Density Calculations of an Octahedral Fe Nanocluster for Selective Electrocatalytic for Nitrogen Reduction. *ACS Applied Nano Materials*, **2021**, 4, 7758-7770	5.6	3
180	Synthesis of 1-indolyl-3,5,8-substituted □carbolines: one-pot solvent-free protocol and biological evaluation. *Beilstein Journal of Organic Chemistry*, **2021**, 17, 1453-1463	2.5	1
179	Dual-functionalization actuated trimodal attribute in an ultra-robust MOF: exceptionally selective capture and effectual fixation of CO2 with fast-responsive, nanomolar detection of assorted organo-contaminants in water. *Materials Chemistry Frontiers*, **2021**, 5, 979-994	7.8	17
178	Computational insights into electrocatalytic CO2 reduction facilitated by Mn(I) half sandwich-based catalysts: Role of substitution and solvent. *Electrochimica Acta*, **2021**, 366, 137463	6.7	0
177	Computational strategies to address the catalytic activity of nanoclusters. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1508	7.9	4
176	Unraveling the catalytically preferential pathway between the direct and indirect hydrogenation of CO2 to CH3OH using N-heterocyclic carbene-based Mn(I) catalysts: a theoretical approach. *Catalysis Science and Technology*, **2021**, 11, 1375-1385	5.5	4
175	Recent Trends in Electrode and Electrolyte Design for Aluminum Batteries. *ACS Omega*, **2021**, 6, 1043-1053	5.9	7
174	Organic cation (DMPI) intercalated graphite anode for high voltage next generation dual-ion batteries. *Materials Advances*, **2021**, 2, 5213-5223	3.3	1

173	Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. *ACS Applied Electronic Materials*, **2021**, 3, 733-742	4	5
172	High-Performance Water Harvester Framework for Triphasic and Synchronous Detection of Assorted Organotoxins with Site-Memory-Reliant Security Encryption via pH-Triggered Fluoroswitching. *ACS Applied Materials & Interfaces*, **2021**, 13, 34012-34026	9.5	13
171	Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. *Journal of Computational Chemistry*, **2021**, 42, 1944-1958	3.5	1
170	Electronic Conductance and Current Modulation through Graphdiyne Nanopores for DNA Sequencing. *ACS Applied Electronic Materials*, **2021**, 3, 3835-3845	4	4
169	Dimensional-Dependent Effects in Platinum Core–Shell-Based Catalysts for Fuel Cell Applications. *ACS Applied Nano Materials*, **2021**, 4, 9697-9708	5.6	1
168	Identifying the preferential pathways of CO capture and hydrogenation to methanol over an Mn(I)-PNP catalyst: a computational study. *Dalton Transactions*, **2021**, 50, 9598-9609	4.3	1
167	Extended topological line defects in graphene for individual identification of DNA nucleobases. *Materials Advances*, **2020**, 1, 2908-2916	3.3	5
166	Unique Dirac and triple point fermiology in simple transition metals and their binary alloys. *Physical Review B*, **2020**, 101,	3.3	3
165	Theoretical Insights into Solid Electrolyte Interphase Formation in an Al Anode Dual-Ion Battery. *Journal of Physical Chemistry C*, **2020**, 124, 7634-7643	3.8	5
164	Identifying suitable ionic liquid electrolytes for Al dual-ion batteries: role of electrochemical window, conductivity and voltage. *Materials Advances*, **2020**, 1, 1354-1363	3.3	9
163	Porphyrin nanoribbon-based spin filtering devices. *Physical Chemistry Chemical Physics*, **2020**, 22, 16368-16377	3.6	1
162	Prospects of black phosphorus nanoribbon for explosive sensing: A computational approach. *Applied Surface Science*, **2020**, 529, 147094	6.7	9
161	Size Evolution Dynamics of Gold Nanoclusters at an Atom-Precision Level: Ligand Exchange, Growth Mechanism, Electrochemical, and Photophysical Properties. *Journal of Physical Chemistry Letters*, **2020**, 11, 1781-1788	6.4	13
160	Unusual demetalation of iron from [2]ferrocenophane skeleton of di-nuclear ferracycle carbonyl complex. *Applied Organometallic Chemistry*, **2020**, 34, e5431	3.1	
159	Theoretical Insights into the Charge and Discharge Processes in Aluminum–Sulfur Batteries. *Journal of Physical Chemistry C*, **2020**, 124, 11317-11324	3.8	8
158	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. *Nanoscale Advances*, **2020**, 2, 2410-2421	5.1	5
157	Temperature-induced crystallinity and vibrational properties in samarium orthovanadate. *Physical Review B*, **2020**, 101,	3.3	5
156	Symmetry-driven topological phases in XAgBi (X=Ba,Sr): An ab initio hybrid functional calculation. *Physical Review Materials*, **2020**, 4,	3.2	4

155	First principles investigation on the applicability of ruthenium as a potential ORR catalyst. *Journal of Chemical Sciences*, **2020**, 132, 1	1.8	4
154	Serendipitous base catalysed condensation-heteroannulation of iminoesters: a regioselective route to the synthesis of 4,6-disubstituted 5-azaindoles. *Organic and Biomolecular Chemistry*, **2020**, 18, 1582-1587	3.9	4
153	Novel BCN-phosphorene bilayer: Dependence of carbon doping on band offsets for potential photovoltaic applications. *Applied Surface Science*, **2020**, 504, 144327	6.7	6
152	Functionalized carbon nanotube electrodes for controlled DNA sequencing. *Nanoscale Advances*, **2020**, 2, 4041-4050	5.1	9
151	Defects Engineering on Ceria and C-C Coupling Reactions Using [Au(PPh)I] Nanocluster: A Combined Experimental and Theoretical Study. *ACS Nano*, **2020**,	16.7	6
150	Superior anchoring effect of a Cu-benzenehexathial MOF as an aluminium–sulfur battery cathode host. *Materials Advances*, **2020**, 1, 3572-3581	3.3	4
149	Individual Identification of Amino Acids on an Atomically Thin Hydrogen Boride System Using Electronic Transport Calculations. *Journal of Physical Chemistry C*, **2020**, 124, 27194-27202	3.8	4
148	Synergistic Effect of Bridging Thiolate and Hub Atoms for the Aromaticity Driven Symmetry Breaking in Atomically Precise Gold Nanocluster. *Journal of Physical Chemistry Letters*, **2020**, 11, 10052-10059	6.4	2
147	Symmetry protection and giant Fermi arcs from multifold fermions in binary, ternary, and quaternary compounds. *Physical Review B*, **2020**, 102,	3.3	3
146	Au-Seeded Ag-Nanorod Networks for Electrocatalytic Sensing. *ACS Applied Nano Materials*, **2020**, 3, 9969-9983	5.9	3
145	Elucidating Mechanistic Origin of the Catalytic Activity of the Fe(111) Surface and Nanoclusters toward the Electrochemical Nitrogen Reduction Reaction. *Journal of Physical Chemistry C*, **2020**, 124, 20193-20202	3.8	3
144	BCN monolayer for high capacity Al-based dual-ion batteries. *Materials Advances*, **2020**, 1, 2418-2425	3.3	3
143	Computational insights into selective CO2 hydrogenation to CH3OH catalysed by ZnO based nanocages. *Materials Advances*, **2020**, 1, 2300-2309	3.3	5
142	Electronic Transport through DNA Nucleotides in BC3 Nanogap for Rapid DNA Sequencing. *ACS Applied Electronic Materials*, **2020**, 2, 1218-1225	4	10
141	Computational Insights into the Working Mechanism of the LiPF6–Graphite Dual-Ion Battery. *Journal of Physical Chemistry C*, **2019**, 123, 23863-23871	3.8	12
140	Density Functional Theory Study of Defect Induced Ferromagnetism and Half-Metallicity in CaI2 Based Monolayer for Spintronics Applications. *ACS Applied Nano Materials*, **2019**, 2, 6152-6161	5.6	10
139	Recent Advances in Graphene-like 2D Materials for Spintronics Applications. *Chemistry of Materials*, **2019**, 31, 8260-8285	9.6	60
138	Graphene/hBN Heterostructures as High-Capacity Cathodes with High Voltage for Next-Generation Aluminum Batteries. *Journal of Physical Chemistry C*, **2019**, 123, 3959-3967	3.8	26

137	Emergence of Topological insulator and Nodal line semi-metal states in XXPBi (X = Na, K, Rb, Cs; XP= Ca, Sr). *Scientific Reports*, **2019**, 9, 527	4.9	7
136	Quaternary Heusler alloy: An ideal platform to realize triple point fermions. *Physical Review B*, **2019**, 99,	3.3	14
135	A computational study on ligand assisted vs. ligand participation mechanisms for CO hydrogenation: importance of bifunctional ligand based catalysts. *Physical Chemistry Chemical Physics*, **2019**, 21, 3932-3941	3.6	12
134	Guest-Induced Ultrasensitive Detection of Multiple Toxic Organics and Fe Ions in a Strategically Designed and Regenerative Smart Fluorescent Metal-Organic Framework. *ACS Applied Materials & Interfaces*, **2019**, 11, 9042-9053	9.5	117
133	Ruthenium-Catalyzed C-H Bond Activation/Arylation Accelerated by Biomass-Derived Ligands. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2844-2852	2.3	1
132	Hexagonal CuCl Monolayer for Water Splitting: A DFT Study. *ACS Applied Nano Materials*, **2019**, 2, 4238-4246	5.6	10
131	Identification of Non-Carbonaceous Cathodes in Al Batteries: Potential Applicability of Black and Blue Phosphorene Monolayers. *Chemistry - an Asian Journal*, **2019**, 14, 2831-2837	4.5	3
130	Spin-Polarized Current in Ferromagnetic Half-Metallic Transition-Metal Iodide Nanowires. *Journal of Physical Chemistry C*, **2019**, 123, 15717-15723	3.8	8
129	Computational Screening of Electrocatalytic Activity of Transition Metal-Doped CdS Nanotubes for Water Splitting. *Journal of Physical Chemistry C*, **2019**, 123, 13419-13427	3.8	7
128	Broken symmetry driven phase transitions from a topological semimetal to a gapped topological phase in SrAgAs. *Physical Review B*, **2019**, 99,	3.3	5
127	Catalytic upgrading of ethanol to n-butanol using an aliphatic MnPNP complex: theoretical insights into reaction mechanisms and product selectivity. *Catalysis Science and Technology*, **2019**, 9, 2794-2805	5.5	7
126	Metal-ligand bifunctional based Mn-catalysts for CO2 hydrogenation reaction. *Molecular Catalysis*, **2019**, 468, 109-116	3.3	13
125	Theoretical insights into CO2 hydrogenation to methanol by a MnPNP complex. *Catalysis Science and Technology*, **2019**, 9, 1867-1878	5.5	19
124	Double-Exchange Magnetic Interactions in High-Temperature Ferromagnetic Iron Chalcogenide Monolayers. *ChemPhysChem*, **2019**, 20, 873-880	3.2	3
123	Enhanced Lewis acid-base adducts in doped stanene: Sensing and photocatalysis. *Applied Surface Science*, **2019**, 478, 946-958	6.7	8
122	Individual Identification of DNA Nucleobases on Atomically Thin Black Phosphorene Nanoribbons: van der Waals Corrected Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2019**, 123, 22377-22383	3.8	21
121	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. *Journal of Materials Chemistry A*, **2019**, 7, 19471-19484	13	56
120	Identification of Intermediate Au(SR)(SR)2 Cluster on Ligand-Induced Transformation of Au(SR) Nanocluster. *Journal of Physical Chemistry Letters*, **2019**, 10, 4571-4576	6.4	10

119	Recent advancements in Pt-nanostructure-based electrocatalysts for the oxygen reduction reaction. *Catalysis Science and Technology*, **2019**, 9, 4835-4863	5.5	47
118	Chemical Degradation of Mercury Alkyls Mediated by Copper Selenide Nanosheets. *Chemistry - an Asian Journal*, **2019**, 14, 4582-4587	4.5	2
117	Hexagonal Cu(111) Monolayers for Selective CO2 Hydrogenation to CH3OH: Insights from Density Functional Theory. *ACS Applied Nano Materials*, **2019**, 2, 7686-7695	5.6	8
116	Zone-Specific Crystallization and a Porosity-Directed Scaling Marker for the Catalytic Efficacy of Au□Ag Alloy Nanoparticles. *ACS Applied Nano Materials*, **2019**, 2, 7669-7685	5.6	2
115	Type-II Dirac states in full Heusler compounds XInPd2 (X = Ti, Zr, and Hf). *Physical Review B*, **2019**, 100,	3.3	6
114	Electronic Transport through DNA Nucleotides in Atomically Thin Phosphorene Electrodes for Rapid DNA Sequencing. *ACS Applied Materials & Interfaces*, **2019**, 11, 219-225	9.5	25
113	Role of Dimensionality for Photocatalytic Water Splitting: CdS Nanotube versus Bulk Structure. *ChemPhysChem*, **2019**, 20, 383-391	3.2	14
112	Computational Screening for ORR Activity of 3d Transition Metal Based M@Pt Core□Shell Clusters. *Journal of Physical Chemistry C*, **2019**, 123, 3634-3644	3.8	27
111	A computational study of electrocatalytic CO2 reduction by Mn(I) complexes: Role of bipyridine substituents. *Electrochimica Acta*, **2019**, 297, 606-612	6.7	12
110	Flexible proton-responsive ligand-based Mn(i) complexes for CO hydrogenation: a DFT study. *Physical Chemistry Chemical Physics*, **2018**, 20, 12535-12542	3.6	8
109	Topologically protected hybrid states in graphene□tanene□graphene heterojunctions. *Journal of Materials Chemistry C*, **2018**, 6, 1920-1925	7.1	8
108	Graphene-like Carbon□Nitride Monolayer: A Potential Anode Material for Na- and K-Ion Batteries. *Journal of Physical Chemistry C*, **2018**, 122, 2481-2489	3.8	99
107	Ferromagnetism and Half-Metallicity in a High-Band-Gap Hexagonal Boron Nitride System. *ChemPhysChem*, **2018**, 19, 153-161	3.2	8
106	First-Principles Study of Magnesium Peroxide Nucleation for Mg-Air Battery. *Chemistry - an Asian Journal*, **2018**, 13, 3198-3203	4.5	4
105	Multilayered Platinum Nanotube for Oxygen Reduction in a Fuel Cell Cathode: Origin of Activity and Product Selectivity. *ACS Applied Energy Materials*, **2018**, 1, 3890-3899	6.1	7
104	Electron-rich graphite-like electrode: stability vs. voltage for Al batteries. *Journal of Materials Chemistry A*, **2018**, 6, 10776-10786	13	20
103	High Curie temperature and half-metallicity in an atomically thin main group-based boron phosphide system: long range ferromagnetism. *Physical Chemistry Chemical Physics*, **2018**, 20, 22877-22889	3.6	18
102	The significance of acid-base properties in the key ligand for (hbox {CO}_{2}) hydrogenation: role of amido ligand. *Journal of Chemical Sciences*, **2018**, 130, 1	1.8	2

101	Zn(II)-nucleobase metal-organic nanofibers and nanoflowers: synthesis and photocatalytic application. *New Journal of Chemistry*, **2018**, 42, 17983-17990	3.6	10
100	Ferromagnetism in magnesium chloride monolayer with an unusually large spin-up gap. *Nanoscale*, **2018**, 10, 22280-22292	7.7	13
99	Topologically nontrivial phase in the hexagonal antiperovskites A3BiB (A=Ba,Sr; B=P,N). *Physical Review B*, **2018**, 98,	3.3	3
98	High-energy-density dual-ion battery for stationary storage of electricity using concentrated potassium fluorosulfonylimide. *Nature Communications*, **2018**, 9, 4469	17.4	140
97	Crystal-defect-induced facet-dependent electrocatalytic activity of 3D gold nanoflowers for the selective nanomolar detection of ascorbic acid. *Nanoscale*, **2018**, 10, 11091-11102	7.7	12
96	Protection of Endogenous Thiols against Methylmercury with Benzimidazole-Based Thione by Unusual Ligand-Exchange Reactions. *Chemistry - A European Journal*, **2017**, 23, 5696-5707	4.8	21
95	The staging mechanism of AlCl intercalation in a graphite electrode for an aluminium-ion battery. *Physical Chemistry Chemical Physics*, **2017**, 19, 7980-7989	3.6	104
94	A free-standing platinum monolayer as an efficient and selective catalyst for the oxygen reduction reaction. *Journal of Materials Chemistry A*, **2017**, 5, 5303-5313	13	25
93	A Computational Study of a Single-Walled Carbon-Nanotube-Based Ultrafast High-Capacity Aluminum Battery. *Chemistry - an Asian Journal*, **2017**, 12, 1944-1951	4.5	16
92	Hexagonal BC3 Electrode for a High-Voltage Al-Ion Battery. *Journal of Physical Chemistry C*, **2017**, 121, 9748-9756	3.8	27
91	Bimetallic core-based cuboctahedral core-shell nanoclusters for the formation of hydrogen peroxide (2e reduction) over water (4e reduction): role of core metals. *Nanoscale*, **2017**, 9, 9537-9547	7.7	13
90	Aliphatic Mn-PNP complexes for the CO2 hydrogenation reaction: a base free mechanism. *Catalysis Science and Technology*, **2017**, 7, 3234-3242	5.5	23
89	Thermochemical and electrochemical CO 2 reduction on octahedral Cu nanocluster: Role of solvent towards product selectivity. *Journal of Catalysis*, **2017**, 349, 118-127	7.3	37
88	Room-Temperature Magneto-dielectric Effect in LaGaFeO; Origin and Impact of Excess Oxygen. *Inorganic Chemistry*, **2017**, 56, 3809-3819	5.1	11
87	Band gap opening in stanene induced by patterned B-N doping. *Physical Chemistry Chemical Physics*, **2017**, 19, 3660-3669	3.6	41
86	Exploiting Le Chatelier's principle for a one-pot synthesis of nontoxic HHogGNPs with the sharpest nanoscopic features suitable for tunable plasmon spectroscopy and high throughput SERS sensing. *Chemical Communications*, **2017**, 53, 10402-10405	5.8	7
85	Stanene based gas sensors: effect of spin-orbit coupling. *Physical Chemistry Chemical Physics*, **2017**, 19, 31325-31334	3.6	37
84	Ferromagnetism and Half-Metallicity in Atomically Thin Holey Nitrogenated Graphene Based Systems. *ChemPhysChem*, **2017**, 18, 2336-2346	3.2	11

83	Effect on catecholase activity and interaction with biomolecules of metal complexes containing differently tuned 5-substituted ancillary tetrazolato ligands. *Polyhedron*, **2017**, 121, 155-171	2.7	5
82	Semiconducting phase in borophene: role of defect and strain. *Journal Physics D: Applied Physics*, **2017**, 50, 405103	3	12
81	TM@gt-C3N3 monolayers: high-temperature ferromagnetism and high anisotropy. *Journal of Materials Chemistry C*, **2016**, 4, 8253-8262	7.1	20
80	Catalytic Hydrogenation of CO2 by Manganese Complexes: Role of Acceptor Ligands. *Journal of Physical Chemistry C*, **2016**, 120, 16478-16488	3.8	34
79	Fe doped LaGaO3: good white light emitters. *RSC Advances*, **2016**, 6, 100230-100238	3.7	27
78	Catalytic Hydrogenation of CO2 by Fe Complexes Containing Pendant Amines: Role of Water and Base. *Journal of Physical Chemistry C*, **2016**, 120, 26652-26662	3.8	15
77	Metal-free half-metallicity in a high energy phase C-doped gh-C3N4 system: a high Curie temperature planar system. *Journal of Materials Chemistry C*, **2016**, 4, 11530-11539	7.1	26
76	Octahedral Ni-nanocluster (Ni85) for Efficient and Selective Reduction of Nitric Oxide (NO) to Nitrogen (N2). *Scientific Reports*, **2016**, 6, 25590	4.9	13
75	Transition-metal embedded carbon nitride monolayers: high-temperature ferromagnetism and half-metallicity. *Nanoscale*, **2016**, 8, 14117-26	7.7	42
74	Coordination polymer hydrogels through Ag(I)-mediated spontaneous self-assembly of unsubstituted nucleobases and their antimicrobial activity. *RSC Advances*, **2016**, 6, 62968-62973	3.7	28
73	First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage. *International Journal of Hydrogen Energy*, **2016**, 41, 14437-14446	6.7	42
72	Single-layered platinum nanocage: a highly selective and efficient catalyst for fuel cells. *Journal of Materials Chemistry A*, **2016**, 4, 12756-12767	13	28
71	Troponate/Aminotroponate Ruthenium-Arene Complexes: Synthesis, Structure, and Ligand-Tuned Mechanistic Pathway for Direct C-H Bond Arylation with Aryl Chlorides in Water. *Inorganic Chemistry*, **2016**, 55, 6739-49	5.1	16
70	Hexagonal Planar CdS Monolayer Sheet for Visible Light Photocatalysis. *Journal of Physical Chemistry C*, **2016**, 120, 7052-7060	3.8	96
69	Lewis AcidBase Adducts for Improving the Selectivity and Sensitivity of Graphene Based Gas Sensors. *ACS Sensors*, **2016**, 1, 451-459	9.2	23
68	Kinetics behind a Strategy for Modulation of Sustainable Benzoxazines: Experimental Study and Its Theoretical Verification. *Macromolecular Chemistry and Physics*, **2016**, 217, 1342-1353	2.6	12
67	Access to highly active NiPd bimetallic nanoparticle catalysts for C coupling reactions. *Catalysis Science and Technology*, **2016**, 6, 5567-5579	5.5	54
66	N-Heterocylic Carbene-Based Mn Electrocatalyst for Two-Electron CO2Reduction over Proton Reduction. *Journal of Physical Chemistry C*, **2016**, 120, 8821-8831	3.8	34

65	Role of Ti doping and Al and B vacancies in the dehydrogenation of Al(BH4)3. *Journal of Chemical Sciences*, **2016**, 128, 1651-1662	1.8	2
64	An atomically thin ferromagnetic half-metallic pyrazine-fused Mn-porphyrin sheet: a slow spin relaxation system. *Journal of Materials Chemistry C*, **2016**, 4, 9069-9077	7.1	14
63	Copper complexes with a flexible piperazinyl arm: nuclearity driven catecholase activity and interactions with biomolecules. *Journal of Coordination Chemistry*, **2016**, 69, 3619-3637	1.6	11
62	Cuboctahedral vs. octahedral platinum nanoclusters: insights into the shape-dependent catalytic activity for fuel cell applications. *Catalysis Science and Technology*, **2016**, 6, 7913-7923	5.5	19
61	Pt3Ti (Ti19@Pt60)-Based Cuboctahedral Core–Shell Nanocluster Favors a Direct over Indirect Oxygen Reduction Reaction. *ACS Energy Letters*, **2016**, 1, 797-805	20.1	26
60	A cuboctahedral platinum (Pt79) nanocluster enclosed by well defined facets favours di-sigma adsorption and improves the reaction kinetics for methanol fuel cells. *Nanoscale*, **2015**, 7, 13438-51	7.7	14
59	Targeted water soluble copper-tetrazolate complexes: interactions with biomolecules and catecholase like activities. *Dalton Transactions*, **2015**, 44, 20154-67	4.3	41
58	Star shaped ferrocenyl substituted triphenylamines. *RSC Advances*, **2015**, 5, 71046-71051	3.7	8
57	B: Highly Sensitive and Selective Gas Sensor. *Journal of Physical Chemistry C*, **2015**, 119, 24827-24836	3.8	87
56	Cardanol benzoxazines Interplay of oxazine functionality (mono to tetra) and properties. *RSC Advances*, **2015**, 5, 78071-78080	3.7	67
55	Innenrücktitelbild: Chemical Detoxification of Organomercurials (Angew. Chem. 32/2015). *Angewandte Chemie*, **2015**, 127, 9551-9551	3.6	
54	Chemical Detoxification of Organomercurials. *Angewandte Chemie*, **2015**, 127, 9455-9459	3.6	17
53	Chemical Detoxification of Organomercurials. *Angewandte Chemie - International Edition*, **2015**, 54, 9323-7	16.4	31
52	Room-temperature chemoselective reduction of nitro groups using non-noble metal nanocatalysts in water. *Inorganic Chemistry*, **2014**, 53, 2904-9	5.1	92
51	Band gap engineering in huge-gap semiconductor SrZrO3 for visible-light photocatalysis. *International Journal of Hydrogen Energy*, **2014**, 39, 2042-2048	6.7	51
50	Direct vs. indirect pathway for nitrobenzene reduction reaction on a Ni catalyst surface: a density functional study. *Physical Chemistry Chemical Physics*, **2014**, 16, 26365-74	3.6	81
49	Limiting nuclearity in formation of polynuclear metal complexes through [2 + 3] cycloaddition: synthesis and magnetic properties of tri- and pentanuclear metal complexes. *Dalton Transactions*, **2014**, 43, 8083-93	4.3	13
48	The effect of remote substitution on the formation of preferential isomers of cobalt(III)-tetrazolate complexes by microwave assisted cycloaddition. *Inorganic Chemistry Frontiers*, **2014**, 1, 599-610	6.8	8

47	Additives in protic–hydridic hydrogen storage compounds: a molecular study. *RSC Advances*, **2014**, 4, 52785-52795	3.7	1
46	Stereoselective synthesis of highly functionalized tetrahydrocarbazoles through a domino Michael–Henry reaction: an easy access to four contiguous chiral centers. *RSC Advances*, **2013**, 3, 10644	3.7	26
45	Layered Perovskite Sr2Ta2O7 for Visible Light Photocatalysis: A First Principles Study. *Journal of Physical Chemistry C*, **2013**, 117, 5043-5050	3.8	41
44	Cationic-anionic mediated charge compensation on La2Ti2O7 for visible light photocatalysis. *Physical Chemistry Chemical Physics*, **2013**, 15, 17150-7	3.6	19
43	Anion-Doped NaTaO3 for Visible Light Photocatalysis. *Journal of Physical Chemistry C*, **2013**, 117, 22518-22524	3.8	63
42	Structural and electrochemical aspects of tris(ferrocenyl/phenyl-ethynyl)phosphine ligated chalcogen bridged iron carbonyl clusters. *RSC Advances*, **2013**, 3, 26025	3.7	11
41	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. *Journal of Catalysis*, **2013**, 299, 204-209	7.3	101
40	Energetic and structural analysis of N2H4BH3 inorganic solid and its modified material for hydrogen storage. *International Journal of Hydrogen Energy*, **2013**, 38, 6718-6725	6.7	6
39	Metal-decorated graphene oxide for ammonia adsorption. *Europhysics Letters*, **2013**, 103, 28007	1.6	14
38	The effect of remote substitution on formation of preferential geometrical isomer of cobalt(III)–tetrazolato complexes formed via [2 + 3] cycloaddition. *Inorganic Chemistry Communication*, **2013**, 34, 62-67	3.1	8
37	Anion–Anion Mediated Coupling in Layered Perovskite La2Ti2O7 for Visible Light Photocatalysis. *Journal of Physical Chemistry C*, **2013**, 117, 13845-13852	3.8	39
36	Formation of (E)-[FcC(PS2(OR)2) CH(PS2(OR)2)] (R = Me, Et, Pr) in photolytic reactions of ferrocenylacetylene and [(RO)2PS2H] in hexane/alcohols: Experimental and DFT study. *Journal of Organometallic Chemistry*, **2013**, 748, 46-50	2.3	2
35	Theoretical Study of Electronic Transport through DNA Nucleotides in a Double-Functionalized Graphene Nanogap. *Journal of Physical Chemistry C*, **2013**, 117, 15421-15428	3.8	74
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3	Condensed two- and three-dimensional aromatic systems: a theoretical study on the relative stabilities of isomers of CB19H16+, B20H15Cl, and B20H14Cl2 and comparison to B12H10Cl22-, C6H4Cl2, C10H7Cl, and C10H6Cl2. *Inorganic Chemistry*, **2005**, 44, 7184-8	5.1	6
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