

Srimanta Pakhira

List of Publications by Year in descending order

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53
papers

1,517
citations

304368

22
h-index

329751

37
g-index

54
all docs

54
docs citations

54
times ranked

2022
citing authors

#	ARTICLE	IF	CITATIONS
1	S-Doped MoP Nanoporous Layer Toward High-Efficiency Hydrogen Evolution in pH-Universal Electrolyte. ACS Catalysis, 2019, 9, 651-659.	5.5	167
2	Low-temperature Synthesis of Heterostructures of Transition Metal Dichalcogenide Alloys ($W_xMo_{1-x}S_2$) and Graphene with Superior Catalytic Performance for Hydrogen Evolution. ACS Nano, 2017, 11, 5103-5112.	7.3	157
3	Apically Dominant Mechanism for Improving Catalytic Activities of N-Doped Carbon Nanotube Arrays in Rechargeable Zinc-Air Battery. Advanced Energy Materials, 2018, 8, 1800480.	10.2	153
4	Achieving Fast and Efficient K^+ Intercalation on Ultrathin Graphene Electrodes Modified by a Li^+ Based Solid-Electrolyte Interphase. Journal of the American Chemical Society, 2018, 140, 13599-13603.	6.6	54
5	Hybridization of Co_3O_4 and \pm -MnO ₂ Nanostructures for High-Performance Nonenzymatic Glucose Sensing. ACS Sustainable Chemistry and Engineering, 2018, 6, 13248-13261.	3.2	54
6	Iron Intercalation in Covalent-Organic Frameworks: A Promising Approach for Semiconductors. Journal of Physical Chemistry C, 2017, 121, 21160-21170.	1.5	46
7	Modulating Electrocatalysis on Graphene Heterostructures: Physically Impermeable Yet Electronically Transparent Electrodes. ACS Nano, 2018, 12, 2980-2990.	7.3	45
8	Large and Uniform Single Crystals of MoS_2 Monolayers for ppb-Level NO_2 Sensing. ACS Applied Nano Materials, 2022, 5, 9415-9426.	2.4	44
9	Synthesis and Characterization of Tris-chelate Complexes for Understanding f -Orbital Bonding in Later Actinides. Journal of the American Chemical Society, 2019, 141, 2356-2366.	6.6	41
10	Constructing a High-Performance Aqueous Rechargeable Zinc-Ion Battery Cathode with Self-Assembled Mat-like Packing of Intertwined Ag(I) Pre-Inserted $V_3O_7 \cdot 2H_2O$ Microbelts with Reduced Graphene Oxide Core. ACS Sustainable Chemistry and Engineering, 2021, 9, 3985-3995.	3.2	40
11	Diverse Rotational Flexibility of Substituted Dicarboxylate Ligands in Functional Porous Coordination Polymers. Journal of Physical Chemistry C, 2015, 119, 28789-28799.	1.5	31
12	Tuning the Dirac Cone of Bilayer and Bulk Structure Graphene by Intercalating First Row Transition Metals Using First-Principles Calculations. Journal of Physical Chemistry C, 2018, 122, 4768-4782.	1.5	30
13	Rapidly Reversible Organic Crystalline Switch for Conversion of Heat into Mechanical Energy. Journal of the American Chemical Society, 2021, 143, 5951-5957.	6.6	29
14	A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. Journal of Physical Chemistry A, 2015, 119, 4214-4223.	1.1	28
15	Intercalation of first row transition metals inside covalent-organic frameworks (COFs): a strategy to fine tune the electronic properties of porous crystalline materials. Physical Chemistry Chemical Physics, 2019, 21, 8785-8796.	1.3	28
16	Raman and electrical transport properties of few-layered arsenic-doped black phosphorus. Nanoscale, 2019, 11, 18449-18463.	2.8	27
17	Catalyzing the Intercalation Storage Capacity of Aqueous Zinc-Ion Battery Constructed with Zn(II) Preinserted Organo-Vanadyl Hybrid Cathode. ACS Applied Energy Materials, 2020, 3, 3425-3434.	2.5	27
18	Mechanism of electrochemical oxygen reduction reaction at two-dimensional Pt-doped $MoSe_2$ material: an efficient electrocatalyst. Journal of Materials Chemistry C, 2021, 9, 11331-11342.	2.7	27

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19	Demystifying the Mechanism of Regio- and Ioselective Epoxide Polymerization Using the Vandenberg Catalyst. <i>Macromolecules</i> , 2018, 51, 1777-1786.	2.2	26
20	Tunability of the Electronic Properties of Covalent Organic Frameworks. <i>ACS Applied Electronic Materials</i> , 2021, 3, 720-732.	2.0	26
21	Performance of dispersion-corrected double hybrid density functional theory: A computational study of OCS-hydrocarbon van der Waals complexes. <i>Journal of Chemical Physics</i> , 2013, 138, 164319.	1.2	25
22	Rotational dynamics of the organic bridging linkers in metal-organic frameworks and their substituent effects on the rotational energy barrier. <i>RSC Advances</i> , 2019, 9, 38137-38147.	1.7	24
23	Recent advancements of two-dimensional transition metal dichalcogenides and their applications in electrocatalysis and energy storage. <i>Emergent Materials</i> , 2021, 4, 951-970.	3.2	24
24	Energy framework approach to the supramolecular reactions: interplay of the secondary bonding interaction in Ph_2E_2 ($\text{E} = \text{Se}, \text{Te}$)- $\text{I-C}_6\text{F}_4$ -I co-crystals. <i>New Journal of Chemistry</i> , 2019, 43, 7941-7949.	1.4	22
25	Quantum Monte Carlo Study of the Reactions of CH with Acrolein: Major and Minor Channels. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3602-3612.	1.1	21
26	Unveiling the role of 2D monolayer Mn-doped MoS_2 material: toward an efficient electrocatalyst for H_2 evolution reaction. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 265-280.	1.3	21
27	Dirac cone in two dimensional bilayer graphene by intercalation with V, Nb, and Ta transition metals. <i>Journal of Chemical Physics</i> , 2018, 148, 064707.	1.2	20
28	A Computational Study of Detoxification of Lewisite Warfare Agents by British Anti-lewisite: Catalytic Effects of Water and Ammonia on Reaction Mechanism and Kinetics. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3496-3506.	1.1	19
29	Can two T-shaped isomers of OCS-C ₂ H ₂ van der Waals complex exist?. <i>Chemical Physics Letters</i> , 2012, 549, 6-11.	1.2	16
30	Dispersion corrected double high-hybrid and gradient-corrected density functional theory study of light cation-dihydrogen (M^+H_2 , where $\text{M} = \text{Li}, \text{Na}, \text{B}$ and Al) van der Waals complexes. <i>Structural Chemistry</i> , 2013, 24, 549-558.	1.0	16
31	Interactions between metal cations with H ₂ in the M^+H_2 complexes: Performance of DFT and DFT-D methods. <i>Journal of Chemical Sciences</i> , 2016, 128, 621-631.	0.7	16
32	Low temperature activation of inert hexagonal boron nitride for metal deposition and single atom catalysis. <i>Materials Today</i> , 2021, 51, 108-116.	8.3	16
33	Spectroscopic properties of $\text{I}_2\text{-Rg}$ ($\text{Rg} = \text{He}, \text{Ne}, \text{Ar}$) van der Waals complexes. <i>Chemical Physics Letters</i> , 2011, 505, 81-86.	1.2	15
34	Reaction mechanism of the selective reduction of CO_2 to CO by a tetraaza $[\text{Co}^{\text{II}}\text{N}_4\text{H}]^{2+}$ complex in the presence of protons. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24058-24064.	1.3	15
35	Spectroscopy and dissociation of $\text{I}_2\text{-Rg}$ ($\text{Rg} = \text{Kr}$ and Xe) van der Waals complexes. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 95-101.	0.5	14
36	Binder-Free ZnO Cathode synthesized via ALD by Direct Growth of Hierarchical ZnO Nanostructure on Current Collector for High-Performance Rechargeable Aluminium-Ion Batteries. <i>ChemistrySelect</i> , 2018, 3, 12512-12523.	0.7	14

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37	Substituents Effects of Organic Linkers on Rotational Energy Barriers in Metal-Organic Frameworks. <i>ChemistrySelect</i> , 2019, 4, 8584-8592.	0.7	14
38	Pyrene-based fluorescent Ru(II)-arene complexes for significant biological applications: catalytic potential, DNA/protein binding, two photon cell imaging and <i>in vitro</i> cytotoxicity. <i>Dalton Transactions</i> , 2022, 51, 3937-3953.	1.6	14
39	Efficient electrocatalytic H ₂ evolution mediated by 2D Janus MoSSe transition metal dichalcogenide. <i>Sustainable Energy and Fuels</i> , 2022, 6, 1733-1752.	2.5	14
40	Quantum Nature in the Interaction of Molecular Hydrogen with Porous Materials: Implications for Practical Hydrogen Storage. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6454-6460.	1.5	12
41	Mechanistic Insight for Targeting Biomolecules by Ruthenium(II) NSAID Complexes. <i>ACS Applied Bio Materials</i> , 2020, 3, 4600-4612.	2.3	11
42	Control of Diffusion and Conformation Behavior of Methyl Methacrylate Monomer by Phenylene Fin in Porous Coordination Polymers. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27291-27297.	1.5	10
43	Theoretical study of spectroscopy, interaction, and dissociation of linear and T-shaped isomers of RgClF (Rg=He, Ne, and Ar) van der Waals complexes. <i>Structural Chemistry</i> , 2012, 23, 681-692.	1.0	8
44	Theoretical study of efficiency of metal cations (Mg ⁺ , Ca ⁺ , and Tl ⁺) in the adsorption of CO ₂ on porous coordination polymers. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27291-27297.	0.8	8
45	Association reaction between SiH ₃ and H ₂ O ₂ : a computational study of the reaction mechanism and kinetics. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	7
46	Structure, stability, and dissociation of small ionic silicon oxide clusters [SiO _n ⁺ (n = 3, 4)]: Insight from density functional and topological exploration. <i>Journal of Chemical Physics</i> , 2013, 139, 234303.	1.2	7
47	H ₂ physisorption on covalent organic framework linkers and metalated linkers: a strategy to enhance binding strength. <i>Molecular Systems Design and Engineering</i> , 2022, 7, 577-591.	1.7	7
48	Selective anticancer activities of ruthenium(II)-tetrazole complexes and their mechanistic insights. <i>BioMetals</i> , 2021, 34, 795-812.	1.8	6
49	Coupled cluster study of structural properties of RgI and RgI ⁺ (Rg=He, Ne, Ar) weakly bound molecules. <i>Structural Chemistry</i> , 2011, 22, 893-900.	1.0	5
50	Binding affinity of substituted ureido-benzenesulfonamide ligands to the carbonic anhydrase receptor: A theoretical study of enzyme inhibition. <i>Journal of Computational Chemistry</i> , 2013, 34, 1907-1916.	1.5	5
51	Hydrogen: A Future Chemical Fuel. <i>Materials Horizons</i> , 2022, , 1-30.	0.3	5
52	Generation of emissive nanosphere from micro-aggregates in anionic perylene diimide: Co-relation of self-assembly, emission, and electrical properties. <i>Dyes and Pigments</i> , 2021, 192, 109461.	2.0	4
53	Electrochemical Water Splitting: H ₂ Evolution Reaction. <i>Materials Horizons</i> , 2022, , 59-89.	0.3	2