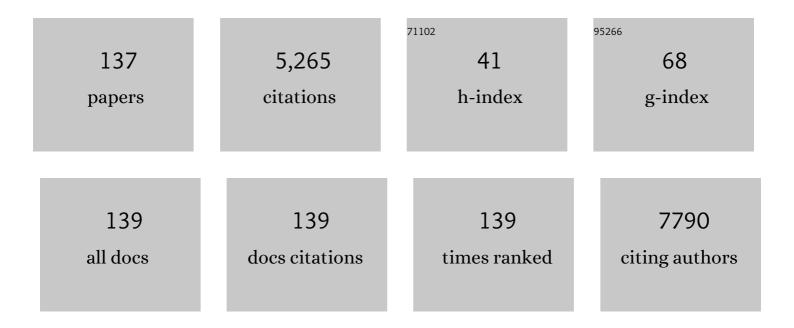
Assistâ€P.rof Sudip Chakraborty

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Defect Engineered g-C ₃ N ₄ for Efficient Visible Light Photocatalytic Hydrogen Production. Chemistry of Materials, 2015, 27, 4930-4933.	6.7	401
2	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. ChemSusChem, 2015, 8, 2789-2825.	6.8	302
3	To Dope Mn ²⁺ in a Semiconducting Nanocrystal. Journal of the American Chemical Society, 2008, 130, 10605-10611.	13.7	237
4	Bi ³⁺ â€Er ³⁺ and Bi ³⁺ â€Yb ³⁺ Codoped Cs ₂ AgInCl ₆ Double Perovskite Nearâ€Infrared Emitters. Angewandte Chemie - International Edition, 2020, 59, 11307-11311.	13.8	223
5	Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. ACS Energy Letters, 2017, 2, 837-845.	17.4	187
6	ns ² Electron (Bi ³⁺ and Sb ³⁺) Doping in Lead-Free Metal Halide Perovskite Derivatives. Chemistry of Materials, 2020, 32, 10255-10267.	6.7	178
7	Highly Sensitive and Selective Gas Detection Based on Silicene. Journal of Physical Chemistry C, 2015, 119, 16934-16940.	3.1	174
8	A possible mechanism for the emergence of an additional band gap due to a Ti–O–C bond in the TiO ₂ –graphene hybrid system for enhanced photodegradation of methylene blue under visible light. RSC Advances, 2014, 4, 59890-59901.	3.6	143
9	Poor Photovoltaic Performance of Cs ₃ Bi ₂ I ₉ : An Insight through First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 17062-17067.	3.1	121
10	Single Atomic Vacancy Catalysis. ACS Nano, 2019, 13, 9958-9964.	14.6	111
11	Na _{2.44} Mn _{1.79} (SO ₄) ₃ : a new member of the alluaudite family of insertion compounds for sodium ion batteries. Journal of Materials Chemistry A, 2015, 3, 18564-18571.	10.3	99
12	Valence Level Character in a Mixed Perovskite Material and Determination of the Valence Band Maximum from Photoelectron Spectroscopy: Variation with Photon Energy. Journal of Physical Chemistry C, 2017, 121, 26655-26666.	3.1	98
13	Synthesis and Optical Properties of Colloidal M ₃ Bi ₂ I ₉ (M = Cs, Rb) Perovskite Nanocrystals. Journal of Physical Chemistry C, 2018, 122, 10643-10649.	3.1	95
14	Nanostructured materials for solid-state hydrogen storage: A review of the achievement of COST Action MP1103. International Journal of Hydrogen Energy, 2016, 41, 14404-14428.	7.1	94
15	Two-dimensional boron: Lightest catalyst for hydrogen and oxygen evolution reaction. Applied Physics Letters, 2016, 109, .	3.3	86
16	Limiting Heterovalent B-Site Doping in CsPbl ₃ Nanocrystals: Phase and Optical Stability. ACS Energy Letters, 2019, 4, 1364-1369.	17.4	86
17	Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. ACS Applied Materials & Interfaces, 2017, 9, 17977-17991.	8.0	82
18	Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. Journal of Physical Chemistry C, 2016, 120, 25256-25262.	3.1	81

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19	Synthesis, structural and electrochemical properties of sodium nickel phosphate for energy storage devices. Nanoscale, 2016, 8, 11291-11305.	5.6	80
20	Rationalizing the Hydrogen and Oxygen Evolution Reaction Activity of Two-Dimensional Hydrogenated Silicene and Germanene. ACS Applied Materials & Interfaces, 2016, 8, 1536-1544.	8.0	69
21	Ionothermal Synthesis of High-Voltage <i>Alluaudite</i> Na _{2+2x} Fe _{2-x} (SO ₄) ₃ Sodium Insertion Compound: Structural, Electronic, and Magnetic Insights. ACS Applied Materials & Interfaces, 2016, 8, 6982-6991.	8.0	66
22	Facets and Defects in Perovskite Nanocrystals for Photocatalytic CO ₂ Reduction. Journal of Physical Chemistry Letters, 2020, 11, 3608-3614.	4.6	64
23	Mechanistic Insight into Enhanced Hydrogen Evolution Reaction Activity of Ultrathin Hexagonal Boron Nitride-Modified Pt Electrodes. ACS Catalysis, 2018, 8, 6636-6644.	11.2	63
24	Cu-doped nickel oxide interface layer with nanoscale thickness for efficient and highly stable printable carbon-based perovskite solar cell. Solar Energy, 2019, 182, 225-236.	6.1	58
25	Understanding the interplay of stability and efficiency in A-site engineered lead halide perovskites. APL Materials, 2020, 8, .	5.1	57
26	Defected and Functionalized Germanene-based Nanosensors under Sulfur Comprising Gas Exposure. ACS Sensors, 2018, 3, 867-874.	7.8	53
27	Na _{2.32} Co _{1.84} (SO ₄) ₃ as a new member of the alluaudite family of high-voltage sodium battery cathodes. Dalton Transactions, 2017, 46, 55-63.	3.3	52
28	A comparative study of hydrogen evolution reaction on pseudo-monolayer WS ₂ and PtS ₂ : insights based on the density functional theory. Catalysis Science and Technology, 2017, 7, 687-692.	4.1	51
29	Solid-state synthesis of stable and color tunable cesium lead halide perovskite nanocrystals and the mechanism of high-performance photodetection in a monolayer MoS ₂ /CsPbBr ₃ vertical heterojunction. Journal of Materials Chemistry C, 2020, 8, 8917-8934.	5.5	51
30	Synthesis, and crystal and electronic structure of sodium metal phosphate for use as a hybrid capacitor in non-aqueous electrolyte. Dalton Transactions, 2015, 44, 20108-20120.	3.3	50
31	Tweaking Nickel with Minimal Silver in a Heterogeneous Alloy of Decahedral Geometry to Deliver Platinumâ€like Hydrogen Evolution Activity. Angewandte Chemie - International Edition, 2020, 59, 2881-2889.	13.8	50
32	Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage. Nanoscale Advances, 2019, 1, 565-580.	4.6	49
33	Zero-Dimensional Lead-Free Hybrid Perovskite-like Material with a Quantum-Well Structure. Chemistry of Materials, 2019, 31, 1941-1945.	6.7	49
34	Metalâ€Functionalized Silicene for Efficient Hydrogen Storage. ChemPhysChem, 2013, 14, 3463-3466.	2.1	45
35	Functionalization of hydrogenated silicene with alkali and alkaline earth metals for efficient hydrogen storage. Physical Chemistry Chemical Physics, 2013, 15, 18900.	2.8	45
36	Evolution of hydrogen by few-layered black phosphorus under visible illumination. Journal of Materials Chemistry A, 2017, 5, 24874-24879.	10.3	45

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37	Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of CsI and Bil ₃ . Inorganic Chemistry, 2019, 58, 12040-12052.	4.0	45
38	Mono- and co-doped NaTaO ₃ for visible light photocatalysis. Physical Chemistry Chemical Physics, 2014, 16, 16085-16094.	2.8	44
39	Substitution induced band structure shape tuning in hybrid perovskites (CH ₃ NH ₃ Pb _{1â°x} Sn _x I ₃) for efficient solar cell applications. RSC Advances, 2015, 5, 107497-107502.	3.6	44
40	In pursuit of bifunctional catalytic activity in PdS2 pseudo-monolayer through reaction coordinate mapping. Nano Energy, 2018, 49, 283-289.	16.0	44
41	Molecular and Selfâ€Trapped Excitonic Contributions to the Broadband Luminescence in Diamineâ€Based Lowâ€Dimensional Hybrid Perovskite Systems. Advanced Optical Materials, 2018, 6, 1800751.	7.3	43
42	Na ₂ M ₂ (SO ₄) ₃ (M = Fe, Mn, Co and Ni): towards high-voltage sodium battery applications. Physical Chemistry Chemical Physics, 2016, 18, 9658-9665.	2.8	40
43	Lewis Acid–Base Interactions between Polysulfides and Boehmite Enables Stable Roomâ€Temperature Sodium–Sulfur Batteries. Advanced Functional Materials, 2020, 30, 2005669.	14.9	40
44	Investigation on Organic Molecule Additive for Moisture Stability and Defect Passivation via Physisorption in CH ₃ NH ₃ PbI ₃ Based Perovskite. ACS Applied Energy Materials, 2018, 1, 1870-1877.	5.1	37
45	Unveiling the Roles of Lattice Strain and Descriptor Species on Pt-Like Oxygen Reduction Activity in Pd–Bi Catalysts. ACS Catalysis, 2021, 11, 800-808.	11.2	35
46	Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer. ACS Applied Energy Materials, 2018, 1, 3571-3576.	5.1	32
47	Unveiling the charge migration mechanism in Na ₂ O ₂ : implications for sodium–air batteries. Physical Chemistry Chemical Physics, 2015, 17, 8203-8209.	2.8	30
48	The effect of impurities in ultra-thin hydrogenated silicene and germanene: a first principles study. Physical Chemistry Chemical Physics, 2015, 17, 22210-22216.	2.8	30
49	Design and Control of Cooperativity in Spin-Crossover in Metal–Organic Complexes: A Theoretical Overview. Inorganics, 2017, 5, 47.	2.7	30
50	Enhancement of energy storage capacity of Mg functionalized silicene and silicane under external strain. Applied Physics Letters, 2014, 105, .	3.3	29
51	Maneuvering the Physical Properties and Spin States To Enhance the Activity of La–Sr–Co–Fe–O Perovskite Oxide Nanoparticles in Electrochemical Water Oxidation. ACS Applied Energy Materials, 2018, 1, 3342-3350.	5.1	29
52	Concerted Ion Migration and Diffusionâ€Induced Degradation in Leadâ€Free Ag ₃ Bil ₆ Rudorffite Solar Cells under Ambient Conditions. Solar Rrl, 2021, 5, 2100077.	5.8	28
53	Simultaneous enhancement in charge separation and onset potential for water oxidation in a BiVO ₄ photoanode by W–Ti codoping. Journal of Materials Chemistry A, 2018, 6, 16965-16974.	10.3	27
54	Organic–inorganic hybrid and inorganic halide perovskites: structural and chemical engineering, interfaces and optoelectronic properties. Journal Physics D: Applied Physics, 2021, 54, 133002.	2.8	27

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55	A combined theoretical and experimental approach of a new ternary metal oxide in molybdate composite for hybrid energy storage capacitors. APL Materials, 2018, 6, .	5.1	26
56	Combinatorial Design and Computational Screening of Two-Dimensional Transition Metal Trichalcogenide Monolayers: Toward Efficient Catalysts for Hydrogen Evolution Reaction. Journal of Physical Chemistry Letters, 2020, 11, 3192-3197.	4.6	26
57	TiS ₂ Monolayer as an Emerging Ultrathin Bifunctional Catalyst: Influence of Defects and Functionalization. ChemPhysChem, 2019, 20, 608-617.	2.1	24
58	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS ₃ (A =) Tj ETQqO	0 0 rgBT /C	Overlock 10 Th 24
59	Bi ³⁺ â€Er ³⁺ and Bi ³⁺ â€Yb ³⁺ Codoped Cs ₂ AgInCl ₆ Double Perovskite Nearâ€Infrared Emitters. Angewandte Chemie, 2020, 132, 11403-11407.	2.0	24
60	Revealing an unusual transparent phase of superhard iron tetraboride under high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17050-17053.	7.1	23
61	Mapping Structural Changes in Electrode Materials: Application of the Hybrid Eigenvector-Following Density Functional Theory (DFT) Method to Layered Li _{0.5} MnO ₂ . Chemistry of Materials, 2015, 27, 5550-5561.	6.7	23
62	Shaping a Doped Perovskite Oxide with Measured Grain Boundary Defects to Catalyze Bifunctional Oxygen Activation for a Rechargeable Zn–Air Battery. ACS Applied Materials & Interfaces, 2020, 12, 40355-40363.	8.0	23
63	Improvement in Hydrogen Desorption from β―and γâ€MgH ₂ upon Transitionâ€Metal Doping. ChemPhysChem, 2015, 16, 2557-2561.	2.1	22
64	Probing the pseudo-1-D ion diffusion in lithium titanium niobate anode for Li-ion battery. Physical Chemistry Chemical Physics, 2016, 18, 22323-22330.	2.8	21
65	Predicting electrochemical properties and ionic diffusion in Na _{2+2x} Mn _{2â^x} (SO ₄) ₃ : crafting a promising high voltage cathode material. Journal of Materials Chemistry A, 2016, 4, 451-457.	10.3	21
66	Mechanistic study of Na-ion diffusion and small polaron formation in Kröhnkite Na ₂ Fe(SO ₄) ₂ ·2H ₂ O based cathode materials. Journal of Materials Chemistry A, 2017, 5, 21726-21739.	10.3	18
67	Emergence of Si ₂ BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. ACS Applied Energy Materials, 2019, 2, 8441-8448.	5.1	18
68	Formation of Corrugated <i>n</i> = 1 2D Tin lodide Perovskites and Their Use as Lead-Free Solar Absorbers. ACS Nano, 2021, 15, 6395-6409.	14.6	18
69	Local electrocatalytic activity of PtRu supported on nitrogen-doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy. Journal of Materials Chemistry A, 2021, 9, 21291-21301.	10.3	18
70	Improved sensing characteristics of methane over ZnO nano sheets upon implanting defects and foreign atoms substitution. Nanotechnology, 2017, 28, 415502.	2.6	17
71	Saline Accelerates Oxime Reaction with Aldehyde and Keto Substrates at Physiological pH. Scientific Reports, 2018, 8, 2193.	3.3	17
72	Anisotropic Photoconductivity and Long-Lived Charge Carriers in Bismuth-Based One-Dimensional Perovskite with Type-Ila Band Alignment. Journal of Physical Chemistry Letters, 2020, 11, 6757-6762.	4.6	17

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73	Electronic density-of-states of amorphous vanadium pentoxide films: Electrochemical data and density functional theory calculations. Journal of Applied Physics, 2014, 115, .	2.5	16
74	Designing a new family of oxonium-cation based structurally diverse organic–inorganic hybrid iodoantimonate crystals. Chemical Communications, 2019, 55, 7562-7565.	4.1	16
75	Cationic Effect on Pressure Driven Spin-State Transition and Cooperativity in Hybrid Perovskites. Chemistry of Materials, 2016, 28, 8379-8384.	6.7	15
76	Stable deep blue emission with unity quantum yield in organic–inorganic halide perovskite 2D nanosheets doped with cerium and terbium at high concentrations. Journal of Materials Chemistry C, 2021, 9, 2437-2454.	5.5	15
77	Stabilizing a hexagonal Ru2C via Lifshitz transition under pressure. Applied Physics Letters, 2013, 103, .	3.3	14
78	Cystamine-configured lead halide based 2D hybrid molecular crystals: Synthesis and photoluminescence systematics. APL Materials, 2018, 6, 114204.	5.1	13
79	Current computational trends in polyanionic cathode materials for Li and Na batteries. Journal of Physics Condensed Matter, 2018, 30, 283003.	1.8	13
80	Defect formations and pH-dependent kinetics in kröhnkite Na2Fe(SO4)2·2H2O based cathode for sodium-ion batteries: Resembling synthesis conditions through chemical potential landscape. Nano Energy, 2019, 55, 123-134.	16.0	13
81	High pressure-induced distortion in face-centered cubic phase of thallium. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 11143-11147.	7.1	12
82	Finding the catalytically active sites on the layered tri-chalcogenide compounds CoPS ₃ and NiPS ₃ for hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2021, 23, 23967-23977.	2.8	12
83	Morphologyâ€Tuned Pt ₃ Ge Accelerates Water Dissociation to Industrial‧tandard Hydrogen Production over a wide pH Range. Advanced Materials, 2022, 34, .	21.0	12
84	Optical Properties of Gallium Oxide Clusters from First-Principles Calculations. Journal of Physical Chemistry A, 2012, 116, 10559-10565.	2.5	11
85	Cluster assembly route to a novel octagonal two-dimensional ZnO monolayer. Journal of Physics Condensed Matter, 2017, 29, 335501.	1.8	11
86	Theoretical Evidence behind Bifunctional Catalytic Activity in Pristine and Functionalized Al ₂ C Monolayers. ChemPhysChem, 2018, 19, 148-152.	2.1	11
87	Mapping the sodium intercalation mechanism, electrochemical properties and structural evolution in non-stoichiometric alluaudite Na _{2+2l´} Fe _{2â^l´} (SO ₄) ₃ cathode materials. Journal of Materials Chemistry A, 2019, 7, 17446-17455.	10.3	11
88	High exothermic dissociation in van der Waals like hexagonal two dimensional nitrogene from first–principles molecular dynamics. Applied Surface Science, 2020, 529, 146552.	6.1	11
89	Halide Replacement with Complete Preservation of Crystal Lattice in Mixedâ€Anion Lanthanide Oxyhalides. Angewandte Chemie - International Edition, 2021, 60, 15582-15589.	13.8	11
90	An Organic–Inorganic Perovskitoid with Zwitterion Cysteamine Linker and its Crystal–Crystal Transformation to Ruddlesdenâ€Popper Phase. Angewandte Chemie - International Edition, 2021, 60, 18750-18760.	13.8	11

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91	Progress and challenges in layered two-dimensional hybrid perovskites. Nanotechnology, 2022, 33, 292501.	2.6	11
92	BC ₃ Sheet Functionalized with Lithiumâ€Rich Species Emerging as a Reversible Hydrogen Storage Material. ChemPhysChem, 2015, 16, 634-639.	2.1	9
93	High pressure driven superconducting critical temperature tuning in Sb2Se3 topological insulator. Applied Physics Letters, 2016, 108, 212601.	3.3	9
94	New Concept on Photocatalytic Degradation of Thiophene Derivatives: Experimental and DFT Studies. Journal of Physical Chemistry C, 2018, 122, 15646-15651.	3.1	9
95	Rashba Triggered Electronic and Optical Properties Tuning in Mixed Cation–Mixed Halide Hybrid Perovskites. ACS Applied Energy Materials, 2019, 2, 6990-6997.	5.1	9
96	Probing active sites on MnPSe3 and FePSe3 tri-chalcogenides as a design strategy for better hydrogen evolution reaction catalysts. International Journal of Hydrogen Energy, 2021, 46, 37928-37938.	7.1	9
97	Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space. ACS Omega, 2021, 6, 33240-33252.	3.5	9
98	Probing Photoexcited Charge Carrier Trapping and Defect Formation in Synergistic Doping of SrTiO ₃ . ACS Applied Energy Materials, 2022, 5, 1159-1168.	5.1	9
99	Incorporating Au ₁₁ nanoclusters on MoS ₂ nanosheet edges for promoting the hydrogen evolution reaction at the interface. Nanoscale, 2022, 14, 7919-7926.	5.6	9
100	Bromination-induced stability enhancement with a multivalley optical response signature in guanidinium [C(NH ₂) ₃] ⁺ -based hybrid perovskite solar cells. Journal of Materials Chemistry A, 2017, 5, 18561-18568.	10.3	8
101	Functionalization and Defect-Driven Water Splitting Mechanism on a Quasi-Two-Dimensional TiO2 Hexagonal Nanosheet. ACS Applied Energy Materials, 2019, 2, 5074-5082.	5.1	8
102	N, H Dualâ€Doped Black Anatase TiO ₂ Thin Films toward Significant Selfâ€Activation in Electrocatalytic Hydrogen Evolution Reaction in Alkaline Media. Advanced Energy and Sustainability Research, 2022, 3, 2100137.	5.8	8
103	Reaction coordinate mapping of hydrogen evolution mechanism on Mg3N2 monolayer. International Journal of Hydrogen Energy, 2020, 45, 22848-22854.	7.1	7
104	Self-Assembled Organic Cations-Assisted Band-Edge Tailoring in Bismuth-Based Perovskites for Enhanced Visible Light Absorption and Photoconductivity. Journal of Physical Chemistry Letters, 2021, 12, 5758-5764.	4.6	7
105	Evolution of hybrid organic–inorganic perovskite materials under external pressure. Applied Physics Reviews, 2021, 8, .	11.3	7
106	The Status Quo of Rashba Phenomena in Organic–Inorganic Hybrid Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 361-367.	4.6	7
107	Epitaxial Growth of GaAs Nanowires on Synthetic Mica by Metal–Organic Chemical Vapor Deposition. ACS Applied Materials & Interfaces, 2022, 14, 3395-3403.	8.0	7
108	Electronic and optical properties of agglomerated hydrogen terminated silicon nanoparticles. European Physical Journal D, 2013, 67, 1.	1.3	6

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109	Tweaking Nickel with Minimal Silver in a Heterogeneous Alloy of Decahedral Geometry to Deliver Platinumâ€like Hydrogen Evolution Activity. Angewandte Chemie, 2020, 132, 2903-2911.	2.0	6
110	Enhanced electrocatalytic oxygen evolution activity in geometrically designed SrRuO3 thin films. Applied Surface Science, 2020, 529, 147065.	6.1	6
111	Positive Magnetoresistance in Concentrated γ-CuMn Alloys — An Evidence for Electron–Electron Interaction. International Journal of Modern Physics B, 1998, 12, 2263-2278.	2.0	5
112	Defect Thermodynamics in Nonstoichiometric Alluaudite-Based Polyanionic Materials for Na-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 32856-32868.	8.0	5
113	Emerging piezochromism in transparent lead free perovskite Rb3X2I9 (X = Sb, Bi) under compression: A comparative theoretical insight. Journal of Applied Physics, 2020, 128, 045102.	2.5	5
114	Charge transfer driven interaction of CH4, CO2 and NH3 with TiS2 monolayer: Influence of vacancy defect. Catalysis Today, 2021, 370, 189-195.	4.4	5
115	Structureâ€Tailored Nonâ€Noble Metalâ€based Ternary Chalcogenide Nanocrystals for Ptâ€like Electrocatalytic Hydrogen Production. ChemSusChem, 2021, 14, 3074-3083.	6.8	5
116	Recent Progress in Alâ€, Kâ€, and Znâ€Ion Batteries: Experimental and Theoretical Viewpoints. Energy Technology, 2021, 9, 2100382.	3.8	5
117	Tuning Spin Texture and Spectroscopic Limited Maximum Efficiency through Chemical Composition Space in Double Halide Perovskites. ACS Applied Energy Materials, 2022, 5, 5579-5588.	5.1	5
118	The effect of morphology and confinement on the high-pressure phase transition in ZnO nanostructure. Journal of Applied Physics, 2015, 117, .	2.5	4
119	Rare earth functionalization effect in optical response of ZnO nano clusters. European Physical Journal D, 2016, 70, 1.	1.3	4
120	Role of relativity in high-pressure phase transitions of thallium. Scientific Reports, 2017, 7, 42983.	3.3	4
121	Tuning the Electronic Structure of a Ni-Vacancy-Enriched AuNi Spherical Nanoalloy via Electrochemical Etching for Water Oxidation Studies in Alkaline and Neutral Media. Inorganic Chemistry, 2022, 61, 8570-8584.	4.0	4
122	Composition dependent tuning of electronic and magnetic properties in transition metal substituted Rock-salt MgO. Journal of Magnetism and Magnetic Materials, 2019, 475, 44-53.	2.3	3
123	Structure and energetics of silicon clusters adsorbed on the Au(111) surface: a first principles study. International Journal of Nanotechnology, 2010, 7, 833.	0.2	2
124	Probing defects and their implications in pH-controlled ZnO QDs: a theory-aided experimental investigation. Journal of Materials Science: Materials in Electronics, 2021, 32, 27084-27096.	2.2	2
125	Facile synthesis and phase stability of Cu-based Na ₂ Cu(SO ₄) ₂ · <i>x</i> H ₂ O (<i>x</i> = 0–2) sulfate minerals as conversion type battery electrodes. Dalton Transactions, 2022, 51, 11169-11179.	3.3	2
126	Oxygen impact on quantum confinement effect for silicon clusters in different size regimes: ab initio investigations. European Physical Journal D, 2011, 64, 331-337.	1.3	1

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127	First principles-based adsorption comparison of group IV elements (C, Si, Ge, and Sn) on Au(111)/Ag(111) surface. Journal of Nanoparticle Research, 2012, 14, 1.	1.9	1
128	An ab-initio study of silicon adsorption on metallic surfaces (Au/Ag): Novel perspective to explore chemical bonding. European Physical Journal B, 2012, 85, 1.	1.5	1
129	Time dependent DFT investigation of the optical response in pristine and Gd doped Al2O3. RSC Advances, 2016, 6, 72537-72543.	3.6	1
130	Halide Replacement with Complete Preservation of Crystal Lattice in Mixedâ€Anion Lanthanide Oxyhalides. Angewandte Chemie, 2021, 133, 15710-15717.	2.0	1
131	Tuning composition space in lead-free divalent and tetravalent halide perovskite : a critical review. Emergent Materials, 2022, 5, 1021-1032.	5.7	1
132	Structural and Optical Properties of Oxygenated Silicon Quantum Dots. Advanced Science Letters, 2011, 4, 3580-3584.	0.2	1
133	Ab-Initio Calculation for the Study of Nano Scale Silicon Based Device Structure. Solid State Phenomena, 0, 139, 113-118.	0.3	0
134	Quantum Confinement Effect in Pristine and Oxygen Covered Silicon Nanocrystals with Surface States. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1739-1743.	0.4	0
135	Study of Silicon-metal Interaction in Adsorption Process: An Ab-initio Approach. Materials Research Society Symposia Proceedings, 2011, 1305, 1.	0.1	0
136	An Organic–Inorganic Perovskitoid with Zwitterion Cysteamine Linker and its Crystal–Crystal Transformation to Ruddlesdenâ€Popper Phase. Angewandte Chemie, 2021, 133, 18898-18908.	2.0	0
137	Relative Localization Prediction in Covalent Clusters: An <i>Ab Initio</i> Theory Driven Quest. Advanced Science Letters, 2012, 18, 208-212.	0.2	0