

# Assistâ€™Prof Sudip Chakraborty

## List of Publications by Year in descending order

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137  
papers

5,265  
citations

71102

41  
h-index

95266

68  
g-index

139  
all docs

139  
docs citations

139  
times ranked

7790  
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning composition space in lead-free divalent and tetravalent halide perovskite : a critical review. Emergent Materials, 2022, 5, 1021-1032.	5.7	1
2	N, H Dualâ€Doped Black Anatase TiO<sub>2</sub> 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
3	Epitaxial Growth of GaAs Nanowires on Synthetic Mica by Metalâ€Organic Chemical Vapor Deposition. ACS Applied Materials & Interfaces, 2022, 14, 3395-3403.	8.0	7
4	Progress and challenges in layered two-dimensional hybrid perovskites. Nanotechnology, 2022, 33, 292501.	2.6	11
5	Probing Photoexcited Charge Carrier Trapping and Defect Formation in Synergistic Doping of SrTiO<sub>3</sub>. ACS Applied Energy Materials, 2022, 5, 1159-1168.	5.1	9
6	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
7	Incorporating Au<sub>11</sub> nanoclusters on MoS<sub>2</sub> nanosheet edges for promoting the hydrogen evolution reaction at the interface. Nanoscale, 2022, 14, 7919-7926.	5.6	9
8	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
9	Morphologyâ€Tuned Pt<sub>3</sub>Ge Accelerates Water Dissociation to Industrialâ€Standard Hydrogen Production over a wide pH Range. Advanced Materials, 2022, 34, .	21.0	12
10	Facile synthesis and phase stability of Cu-based Na<sub>2</sub>Cu(SO<sub>4</sub>)<sub>2</sub>Â·xH<sub>2</sub>O (x = 0â€2) sulfate minerals as conversion type battery electrodes. Dalton Transactions, 2022, 51, 11169-11179.	3.3	2
11	Charge transfer driven interaction of CH<sub>4</sub>, CO<sub>2</sub> and NH<sub>3</sub> with TiS<sub>2</sub> monolayer: Influence of vacancy defect. Catalysis Today, 2021, 370, 189-195.	4.4	5
12	Unveiling the Roles of Lattice Strain and Descriptor Species on Pt-Like Oxygen Reduction Activity in Pdâ€Bi Catalysts. ACS Catalysis, 2021, 11, 800-808.	11.2	35
13	Organicâ€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
14	Stable deep blue emission with unity quantum yield in organicâ€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
15	Formation of Corrugated x = 1 2D Tin Iodide Perovskites and Their Use as Lead-Free Solar Absorbers. ACS Nano, 2021, 15, 6395-6409.	14.6	18
16	Halide Replacement with Complete Preservation of Crystal Lattice in Mixedâ€Anion Lanthanide Oxyhalides. Angewandte Chemie, 2021, 133, 15710-15717.	2.0	1
17	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
18	Structureâ€Tailored Nonâ€Noble Metalâ€Based Ternary Chalcogenide Nanocrystals for Ptâ€like Electrocatalytic Hydrogen Production. ChemSusChem, 2021, 14, 3074-3083.	6.8	5

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19	Halide Replacement with Complete Preservation of Crystal Lattice in Mixed Anion Lanthanide Oxyhalides. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15582-15589.	13.8	11
20	An Organic-Inorganic Perovskitoid with Zwitterion Cysteamine Linker and its Crystal Transformation to Ruddlesden-Popper Phase. <i>Angewandte Chemie</i> , 2021, 133, 18898-18908.	2.0	0
21	Recent Progress in Al, K, and Zn Ion Batteries: Experimental and Theoretical Viewpoints. <i>Energy Technology</i> , 2021, 9, 2100382.	3.8	5
22	An Organic-Inorganic Perovskitoid with Zwitterion Cysteamine Linker and its Crystal Transformation to Ruddlesden-Popper Phase. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 18750-18760.	13.8	11
23	Concerted Ion Migration and Diffusion-Induced Degradation in Lead-Free Ag <sub>3</sub> Bi <sub>6</sub> Rudorffite Solar Cells under Ambient Conditions. <i>Solar Rrl</i> , 2021, 5, 2100077.	5.8	28
24	Local electrocatalytic activity of PtRu supported on nitrogen-doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy. <i>Journal of Materials Chemistry A</i> , 2021, 9, 21291-21301.	10.3	18
25	Finding the catalytically active sites on the layered tri-chalcogenide compounds CoPS <sub>3</sub> and NiPS <sub>3</sub> for hydrogen evolution reaction. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 23967-23977.	2.8	12
26	Probing defects and their implications in pH-controlled ZnO QDs: a theory-aided experimental investigation. <i>Journal of Materials Science: Materials in Electronics</i> , 2021, 32, 27084-27096.	2.2	2
27	Probing active sites on MnPSe <sub>3</sub> and FePSe <sub>3</sub> tri-chalcogenides as a design strategy for better hydrogen evolution reaction catalysts. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 37928-37938.	7.1	9
28	Evolution of hybrid organic-inorganic perovskite materials under external pressure. <i>Applied Physics Reviews</i> , 2021, 8, .	11.3	7
29	The Status Quo of Rashba Phenomena in Organic-Inorganic Hybrid Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 361-367.	4.6	7
30	Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space. <i>ACS Omega</i> , 2021, 6, 33240-33252.	3.5	9
31	Tweaking Nickel with Minimal Silver in a Heterogeneous Alloy of Decahedral Geometry to Deliver Platinum-like Hydrogen Evolution Activity. <i>Angewandte Chemie</i> , 2020, 132, 2903-2911.	2.0	6
32	Tweaking Nickel with Minimal Silver in a Heterogeneous Alloy of Decahedral Geometry to Deliver Platinum-like Hydrogen Evolution Activity. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 2881-2889.	13.8	50
33	ns <sup>2</sup> Electron (Bi <sup>3+</sup> and Sb <sup>3+</sup> ) Doping in Lead-Free Metal Halide Perovskite Derivatives. <i>Chemistry of Materials</i> , 2020, 32, 10255-10267.	6.7	178
34	Shaping a Doped Perovskite Oxide with Measured Grain Boundary Defects to Catalyze Bifunctional Oxygen Activation for a Rechargeable Zn-Air Battery. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 40355-40363.	8.0	23
35	Emerging piezochromism in transparent lead free perovskite Rb <sub>3</sub> X <sub>2</sub> I <sub>9</sub> (X = Sb, Bi) under compression: A comparative theoretical insight. <i>Journal of Applied Physics</i> , 2020, 128, 045102.	2.5	5
36	Reaction coordinate mapping of hydrogen evolution mechanism on Mg <sub>3</sub> N <sub>2</sub> monolayer. <i>International Journal of Hydrogen Energy</i> , 2020, 45, 22848-22854.	7.1	7

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37	Anisotropic Photoconductivity and Long-Lived Charge Carriers in Bismuth-Based One-Dimensional Perovskite with Type-IIa Band Alignment. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6757-6762.	4.6	17
38	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite $AZrS_3$ ( $A = Tl, ET, Q, O, Rg, BT$ ). <i>Overlock 10 Tf</i>	5.5	24
39	Lewis Acid-Base Interactions between Polysulfides and Boehmite Enables Stable Room-Temperature Sodium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2020, 30, 2005669.	14.9	40
40	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. <i>Journal of Materials Chemistry C</i> , 2020, 8, 8917-8934.	5.5	51
41	$Bi^{3+}/Er^{3+}$ and $Bi^{3+}/Yb^{3+}$ Codoped $Cs_2AgInCl_6$ Double Perovskite Near-Infrared Emitters. <i>Angewandte Chemie</i> , 2020, 132, 11403-11407.	2.0	24
42	$Bi^{3+}/Er^{3+}$ and $Bi^{3+}/Yb^{3+}$ Codoped $Cs_2AgInCl_6$ Double Perovskite Near-Infrared Emitters. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 11307-11311.	13.8	223
43	Enhanced electrocatalytic oxygen evolution activity in geometrically designed $SrRuO_3$ thin films. <i>Applied Surface Science</i> , 2020, 529, 147065.	6.1	6
44	Understanding the interplay of stability and efficiency in A-site engineered lead halide perovskites. <i>APL Materials</i> , 2020, 8, .	5.1	57
45	High exothermic dissociation in van der Waals like hexagonal two dimensional nitrogene from first-principles molecular dynamics. <i>Applied Surface Science</i> , 2020, 529, 146552.	6.1	11
46	Combinatorial Design and Computational Screening of Two-Dimensional Transition Metal Trichalcogenide Monolayers: Toward Efficient Catalysts for Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3192-3197.	4.6	26
47	Facets and Defects in Perovskite Nanocrystals for Photocatalytic $CO_2$ Reduction. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3608-3614.	4.6	64
48	Single Atomic Vacancy Catalysis. <i>ACS Nano</i> , 2019, 13, 9958-9964.	14.6	111
49	Defect Thermodynamics in Nonstoichiometric Alluaudite-Based Polyanionic Materials for Na-Ion Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 32856-32868.	8.0	5
50	Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of $CsI$ and $BiI_3$ . <i>Inorganic Chemistry</i> , 2019, 58, 12040-12052.	4.0	45
51	Rashba Triggered Electronic and Optical Properties Tuning in Mixed Cation-Mixed Halide Hybrid Perovskites. <i>ACS Applied Energy Materials</i> , 2019, 2, 6990-6997.	5.1	9
52	Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage. <i>Nanoscale Advances</i> , 2019, 1, 565-580.	4.6	49
53	Mapping the sodium intercalation mechanism, electrochemical properties and structural evolution in non-stoichiometric alluaudite $Na_{2+2\delta}Fe_{2\delta}SO_4$ cathode materials. <i>Journal of Materials Chemistry A</i> , 2019, 7, 17446-17455.	10.3	11
54	Designing a new family of oxonium-cation based structurally diverse organo-inorganic hybrid iodoantimonate crystals. <i>Chemical Communications</i> , 2019, 55, 7562-7565.	4.1	16

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55	Functionalization and Defect-Driven Water Splitting Mechanism on a Quasi-Two-Dimensional TiO <sub>2</sub> Hexagonal Nanosheet. ACS Applied Energy Materials, 2019, 2, 5074-5082.	5.1	8
56	Limiting Heterovalent B-Site Doping in CsPbI <sub>3</sub> Nanocrystals: Phase and Optical Stability. ACS Energy Letters, 2019, 4, 1364-1369.	17.4	86
57	Zero-Dimensional Lead-Free Hybrid Perovskite-like Material with a Quantum-Well Structure. Chemistry of Materials, 2019, 31, 1941-1945.	6.7	49
58	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
59	Emergence of Si <sub>2</sub> BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. ACS Applied Energy Materials, 2019, 2, 8441-8448.	5.1	18
60	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
61	Defect formations and pH-dependent kinetics in perovskite Na <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·2H <sub>2</sub> O based cathode for sodium-ion batteries: Resembling synthesis conditions through chemical potential landscape. Nano Energy, 2019, 55, 123-134.	16.0	13
62	TiS <sub>2</sub> Monolayer as an Emerging Ultrathin Bifunctional Catalyst: Influence of Defects and Functionalization. ChemPhysChem, 2019, 20, 608-617.	2.1	24
63	Synthesis and Optical Properties of Colloidal M <sub>3</sub> Bi <sub>2</sub> I <sub>9</sub> (M = Cs, Rb) Perovskite Nanocrystals. Journal of Physical Chemistry C, 2018, 122, 10643-10649.	3.1	95
64	Investigation on Organic Molecule Additive for Moisture Stability and Defect Passivation via Physisorption in CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Based Perovskite. ACS Applied Energy Materials, 2018, 1, 1870-1877.	5.1	37
65	In pursuit of bifunctional catalytic activity in PdS <sub>2</sub> pseudo-monolayer through reaction coordinate mapping. Nano Energy, 2018, 49, 283-289.	16.0	44
66	Saline Accelerates Oxime Reaction with Aldehyde and Keto Substrates at Physiological pH. Scientific Reports, 2018, 8, 2193.	3.3	17
67	Defected and Functionalized Germanene-based Nanosensors under Sulfur Comprising Gas Exposure. ACS Sensors, 2018, 3, 867-874.	7.8	53
68	Theoretical Evidence behind Bifunctional Catalytic Activity in Pristine and Functionalized Al <sub>2</sub> C Monolayers. ChemPhysChem, 2018, 19, 148-152.	2.1	11
69	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
70	Cystamine-configured lead halide based 2D hybrid molecular crystals: Synthesis and photoluminescence systematics. APL Materials, 2018, 6, 114204.	5.1	13
71	Current computational trends in polyanionic cathode materials for Li and Na batteries. Journal of Physics Condensed Matter, 2018, 30, 283003.	1.8	13
72	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

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73	Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer. <i>ACS Applied Energy Materials</i> , 2018, 1, 3571-3576.	5.1	32
74	Molecular and Self-Trapped Excitonic Contributions to the Broadband Luminescence in Diamine-Based Low-Dimensional Hybrid Perovskite Systems. <i>Advanced Optical Materials</i> , 2018, 6, 1800751.	7.3	43
75	Simultaneous enhancement in charge separation and onset potential for water oxidation in a BiVO <sub>4</sub> photoanode by W-Ti codoping. <i>Journal of Materials Chemistry A</i> , 2018, 6, 16965-16974.	10.3	27
76	Mechanistic Insight into Enhanced Hydrogen Evolution Reaction Activity of Ultrathin Hexagonal Boron Nitride-Modified Pt Electrodes. <i>ACS Catalysis</i> , 2018, 8, 6636-6644.	11.2	63
77	New Concept on Photocatalytic Degradation of Thiophene Derivatives: Experimental and DFT Studies. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15646-15651.	3.1	9
78	A comparative study of hydrogen evolution reaction on pseudo-monolayer WS <sub>2</sub> and PtS <sub>2</sub> : insights based on the density functional theory. <i>Catalysis Science and Technology</i> , 2017, 7, 687-692.	4.1	51
79	Role of relativity in high-pressure phase transitions of thallium. <i>Scientific Reports</i> , 2017, 7, 42983.	3.3	4
80	Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. <i>ACS Energy Letters</i> , 2017, 2, 837-845.	17.4	187
81	Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 17977-17991.	8.0	82
82	Evolution of hydrogen by few-layered black phosphorus under visible illumination. <i>Journal of Materials Chemistry A</i> , 2017, 5, 24874-24879.	10.3	45
83	Mechanistic study of Na-ion diffusion and small polaron formation in K <sup>+</sup> hkite Na <sub>2</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·2H <sub>2</sub> O based cathode materials. <i>Journal of Materials Chemistry A</i> , 2017, 5, 21726-21739.	10.3	18
84	Improved sensing characteristics of methane over ZnO nano sheets upon implanting defects and foreign atoms substitution. <i>Nanotechnology</i> , 2017, 28, 415502.	2.6	17
85	Bromination-induced stability enhancement with a multivalley optical response signature in guanidinium [C(NH <sub>2</sub> ) <sub>3</sub> ] <sup>+</sup> -based hybrid perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2017, 5, 18561-18568.	10.3	8
86	Valence Level Character in a Mixed Perovskite Material and Determination of the Valence Band Maximum from Photoelectron Spectroscopy: Variation with Photon Energy. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26655-26666.	3.1	98
87	Poor Photovoltaic Performance of Cs <sub>3</sub> Bi <sub>2</sub> I <sub>9</sub> : An Insight through First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17062-17067.	3.1	121
88	Na <sub>2.32</sub> Co <sub>1.84</sub> (SO <sub>4</sub> ) <sub>3</sub> as a new member of the alluaudite family of high-voltage sodium battery cathodes. <i>Dalton Transactions</i> , 2017, 46, 55-63.	3.3	52
89	Design and Control of Cooperativity in Spin-Crossover in Metal-Organic Complexes: A Theoretical Overview. <i>Inorganics</i> , 2017, 5, 47.	2.7	30
90	Cluster assembly route to a novel octagonal two-dimensional ZnO monolayer. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 335501.	1.8	11

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91	Two-dimensional boron: Lightest catalyst for hydrogen and oxygen evolution reaction. Applied Physics Letters, 2016, 109, .	3.3	86
92	High pressure driven superconducting critical temperature tuning in Sb <sub>2</sub> Se <sub>3</sub> topological insulator. Applied Physics Letters, 2016, 108, 212601.	3.3	9
93	Rare earth functionalization effect in optical response of ZnO nano clusters. European Physical Journal D, 2016, 70, 1.	1.3	4
94	Ionothermal Synthesis of High-Voltage <i>Alluaudite</i> Na <sub>2+2x</sub> Fe <sub>2-x</sub> (SO <sub>4</sub> ) <sub>3</sub> Sodium Insertion Compound: Structural, Electronic, and Magnetic Insights. ACS Applied Materials & Interfaces, 2016, 8, 6982-6991.	8.0	66
95	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
96	Synthesis, structural and electrochemical properties of sodium nickel phosphate for energy storage devices. Nanoscale, 2016, 8, 11291-11305.	5.6	80
97	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
98	Time dependent DFT investigation of the optical response in pristine and Gd doped Al <sub>2</sub> O <sub>3</sub> . RSC Advances, 2016, 6, 72537-72543.	3.6	1
99	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
100	Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. Journal of Physical Chemistry C, 2016, 120, 25256-25262.	3.1	81
101	Cationic Effect on Pressure Driven Spin-State Transition and Cooperativity in Hybrid Perovskites. Chemistry of Materials, 2016, 28, 8379-8384.	6.7	15
102	Na <sub>2</sub> M <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> (M = Fe, Mn, Co and Ni): towards high-voltage sodium battery applications. Physical Chemistry Chemical Physics, 2016, 18, 9658-9665.	2.8	40
103	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
104	Predicting electrochemical properties and ionic diffusion in Na <sub>2+2x</sub> Mn <sub>2x</sub> (SO <sub>4</sub> ) <sub>3</sub> : crafting a promising high voltage cathode material. Journal of Materials Chemistry A, 2016, 4, 451-457.	10.3	21
105	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. ChemSusChem, 2015, 8, 2789-2825.	6.8	302
106	Improvement in Hydrogen Desorption from $\hat{2}\hat{a}\hat{e}$ and $\hat{3}\hat{a}\hat{e}$ MgH <sub>2</sub> upon Transition $\hat{e}$ Metal Doping. ChemPhysChem, 2015, 16, 2557-2561.	2.1	22
107	Substitution induced band structure shape tuning in hybrid perovskites (CH <sub>3</sub> NH <sub>3</sub> Pb <sub>1-x</sub> Sn <sub>x</sub> I <sub>3</sub> ) for efficient solar cell applications. RSC Advances, 2015, 5, 107497-107502.	3.6	44
108	Unveiling the charge migration mechanism in Na <sub>2</sub> O <sub>2</sub> : implications for sodium $\hat{e}$ air batteries. Physical Chemistry Chemical Physics, 2015, 17, 8203-8209.	2.8	30

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109	Mapping Structural Changes in Electrode Materials: Application of the Hybrid Eigenvector-Following Density Functional Theory (DFT) Method to Layered Li <sub>0.5</sub> MnO <sub>2</sub> . Chemistry of Materials, 2015, 27, 5550-5561.	6.7	23
110	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
111	Na <sub>2.44</sub> Mn <sub>1.79</sub> (SO <sub>4</sub> ) <sub>3</sub> : 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
112	Defect Engineered g-C <sub>3</sub> N <sub>4</sub> for Efficient Visible Light Photocatalytic Hydrogen Production. Chemistry of Materials, 2015, 27, 4930-4933.	6.7	401
113	Highly Sensitive and Selective Gas Detection Based on Silicene. Journal of Physical Chemistry C, 2015, 119, 16934-16940.	3.1	174
114	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
115	The effect of morphology and confinement on the high-pressure phase transition in ZnO nanostructure. Journal of Applied Physics, 2015, 117, .	2.5	4
116	BC <sub>3</sub> Sheet Functionalized with Lithium-Rich Species Emerging as a Reversible Hydrogen Storage Material. ChemPhysChem, 2015, 16, 634-639.	2.1	9
117	Enhancement of energy storage capacity of Mg functionalized silicene and silicane under external strain. Applied Physics Letters, 2014, 105, .	3.3	29
118	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
119	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
120	A possible mechanism for the emergence of an additional band gap due to a Ti-O-C bond in the TiO <sub>2</sub> -graphene hybrid system for enhanced photodegradation of methylene blue under visible light. RSC Advances, 2014, 4, 59890-59901.	3.6	143
121	Mono- and co-doped NaTaO <sub>3</sub> for visible light photocatalysis. Physical Chemistry Chemical Physics, 2014, 16, 16085-16094.	2.8	44
122	Electronic and optical properties of agglomerated hydrogen terminated silicon nanoparticles. European Physical Journal D, 2013, 67, 1.	1.3	6
123	Metal-Functionalized Silicene for Efficient Hydrogen Storage. ChemPhysChem, 2013, 14, 3463-3466.	2.1	45
124	Functionalization of hydrogenated silicene with alkali and alkaline earth metals for efficient hydrogen storage. Physical Chemistry Chemical Physics, 2013, 15, 18900.	2.8	45
125	Stabilizing a hexagonal Ru <sub>2</sub> C via Lifshitz transition under pressure. Applied Physics Letters, 2013, 103, .	3.3	14
126	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



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127	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
128	Optical Properties of Gallium Oxide Clusters from First-Principles Calculations. Journal of Physical Chemistry A, 2012, 116, 10559-10565.	2.5	11
129	Relative Localization Prediction in Covalent Clusters: An <I>Ab Initio</I> Theory Driven Quest. Advanced Science Letters, 2012, 18, 208-212.	0.2	0
130	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
131	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
132	Study of Silicon-metal Interaction in Adsorption Process: An Ab-initio Approach. Materials Research Society Symposia Proceedings, 2011, 1305, 1.	0.1	0
133	Structural and Optical Properties of Oxygenated Silicon Quantum Dots. Advanced Science Letters, 2011, 4, 3580-3584.	0.2	1
134	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
135	To Dope Mn<sup>2+</sup> in a Semiconducting Nanocrystal. Journal of the American Chemical Society, 2008, 130, 10605-10611.	13.7	237
136	Positive Magnetoresistance in Concentrated $\hat{I}^3$ -CuMn Alloys â€” An Evidence for Electronâ€”Electron Interaction. International Journal of Modern Physics B, 1998, 12, 2263-2278.	2.0	5
137	Ab-Initio Calculation for the Study of Nano Scale Silicon Based Device Structure. Solid State Phenomena, 0, 139, 113-118.	0.3	0