Saswata Bhattacharya

List of Publications by Year
in descending order

72 papers	1,956 citations	257101 24 h-index	264894 42 g-index
73 all docs	73 docs citations	73 times ranked	2436 citing authors

#	Article	IF	Citations
1	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
2	Transition-Metal Decoration Enhanced Room-Temperature Hydrogen Storage in a Defect-Modulated Graphene Sheet. Journal of Physical Chemistry C, 2010, 114, 10297-10301.	1.5	135
3	Band Gap Engineering in Cs₂(Na_{<i>x</i>}Ag_{1â€“<i>x</i>})BiCl₆ Double Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2019, 10, 5173-5181.	2.1	109
4	GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2246-2264.	2.3	86
5	Stability and Metastability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Mg</mml:mi><mml:mi>M</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 135501.	2.9	72
6	Unraveling the structural and morphological stability of oxygen vacancy engineered leaf-templated CaTiO₃ towards photocatalytic H₂ evolution and N₂ fixation reactions. Journal of Materials Chemistry A, 2021, 9, 17006-17018.	5.2	72
7	A fast and effective approach for reversible wetting-dewetting transitions on ZnO nanowires. Scientific Reports, 2016, 6, 35073.	1.6	41
8	Hydrogen Storage in Ti-Decorated BC₄N Nanotube. Journal of Physical Chemistry C, 2008, 112, 17487-17491.	1.5	37
9	Efficient<i>ab initio</i>schemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. New Journal of Physics, 2014, 16, 123016.	1.2	37
10	Lead-Free Alloyed Double-Perovskite Nanocrystals of Cs₂(Na_{<i>x</i>}Ag_{1â€“<i>x</i>})BiBr₆ with Tunable Band Gap. Journal of Physical Chemistry C, 2021, 125, 1954-1962.	1.5	36
11	Anti-Kubas Type Interaction in Hydrogen Storage on a Li Decorated BHNH Sheet: A First-Principles Based Study. Journal of Physical Chemistry C, 2012, 116, 3840-3844.	1.5	35
12	Enhanced Photocurrent Owing to Shuttling of Charge Carriers across 4-Aminothiophenol-Functionalized MoSe₂â€“CsPbBr₃ Nanohybrids. ACS Applied Materials & Interfaces, 2020, 12, 7317-7325.	4.0	35
13	Exploring semiconductor substrates for silicene epitaxy. Applied Physics Letters, 2013, 103, .	1.5	34
14	Tuning the Wettability of Indium Oxide Nanowires from Superhydrophobic to Nearly Superhydrophilic: Effect of Oxygen-Related Defects. Journal of Physical Chemistry C, 2015, 119, 16026-16032.	1.5	33
15	Role of Defects in Photocatalytic Water Splitting: Monodoped vs Codoped SrTiO₃. Journal of Physical Chemistry C, 2020, 124, 10272-10279.	1.5	32
16	Ti-Decorated BC₄N Sheet: A planar Nanostructure for High-Capacity Hydrogen Storage. Journal of Physical Chemistry C, 2009, 113, 15783-15787.	1.5	31
17	Metal-organic frameworks functionalized smart textiles for adsorptive removal of hazardous aromatic pollutants from ambient air. Journal of Hazardous Materials, 2021, 411, 125056.	6.5	31
18	Understanding the efficient electrocatalytic activities of MoSe₂â€“Cu₂S nanoheterostructures. Journal of Materials Chemistry A, 2021, 9, 9837-9848.	5.2	31

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19	Computational design of nanoclusters by property-based genetic algorithms: Tuning the electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>TiO</mml:mi><mn Physical Review B, 2015, 91, .	1.1	29
20	MoS₂and Janus (MoSSe) based 2D van der Waals heterostructures: emerging direct Z-scheme photocatalysts. Nanoscale Advances, 2021, 3, 2837-2845.	2.2	27
21	Formation of Water Chains on CaO(001): What Drives the 1D Growth?. Journal of Physical Chemistry Letters, 2015, 6, 1204-1208.	2.1	26
22	Selective electrochemical reduction of CO₂ to CO on CuO/In₂O₃ nanocomposites: role of oxygen vacancies. Catalysis Science and Technology, 2019, 9, 5339-5349.	2.1	25
23	Reducing lead toxicity in the methylammonium lead halide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">MAPbI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> : Why Sn substitution should be preferred to Pb vacancy for optimum solar cell efficiency. Physical Review B, 2020, 101, .	1.1	25
24	Optoelectronic Properties of Chalcogenide Perovskites by Many-Body Perturbation Theory. Journal of Physical Chemistry Letters, 2021, 12, 5301-5307.	2.1	25
25	Self energy and excitonic effect in (un)doped TiO₂ anatase: a comparative study of hybrid DFT, GW and BSE to explore optical properties. Journal of Materials Chemistry C, 2019, 7, 14284-14293.	2.7	24
26	Engineering Electronic Structure and Lattice Dynamics to Achieve Enhanced Thermoelectric Performance of Mnâ€“Sb Co-Doped GeTe. Chemistry of Materials, 2021, 33, 3611-3620.	3.2	24
27	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. Physical Review Materials, 2017, 1, .	0.9	24
28	Lithium Calcium Imide [Li2Ca(NH)2] for Hydrogen Storage: Structural and Thermodynamic Properties. Journal of Physical Chemistry B, 2008, 112, 11381-11384.	1.2	21
29	Unraveling the role of vacancies in the potentially promising thermoelectric clathrates<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ba</mml:mi><mml:mn>8</mml:mn></m Physical Review B, 2016, 94, .	1.8	20
30	Innovative Approach to Photo-Chemiresistive Sensing Technology: Surface-Fluorinated SnO₂ for VOC Detection. ACS Applied Materials & Interfaces, 2020, 12, 37320-37329.	4.0	19
31	Stability of non-metal dopants to tune the photo-absorption of TiO2 at realistic temperatures and oxygen partial pressures: A hybrid DFT study. Scientific Reports, 2019, 9, 11427.	1.6	17
32	Electronic Effect in a Ruthenium Catalyst Designed in Nanoporous N-Functionalized Carbon for Efficient Hydrogenation of Heteroarenes. ACS Applied Materials & Interfaces, 2020, 12, 52668-52677.	4.0	17
33	Oxygen vacancy mediated cubic phase stabilization at room temperature in pure nano-crystalline zirconia films: a combined experimental and first-principles based investigation. Physical Chemistry Chemical Physics, 2019, 21, 22482-22490.	1.3	16
34	Unraveling The Origin of Enhanced Field Emission from Irradiated FeCo-SiO₂Nanocomposites: A Combined Experimental and First-Principles Based Study. ACS Applied Materials & Interfaces, 2016, 8, 4994-5001.	4.0	14
35	High-throughput screening to modulate electronic and optical properties of alloyed Cs₂AgBiCl₆ for enhanced solar cell efficiency. JPhys Materials, 2021, 4, 025005.	1.8	14
36	Organogel-assisted porous organic polymer embedding Cu NPs for selectivity control in the semi hydrogenation of alkynes. Nanoscale, 2022, 14, 1505-1519.	2.8	14

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37	Elucidating the origin of magnetic ordering in ferroelectric BaTiO₃₋ <i>d</i> thin film via electronic structure modification. Journal of Physics Condensed Matter, 2019, 31, 205001.	0.7	13
38	Understanding the role of Sn substitution and Pb-â–¡ in enhancing the optical properties and solar cell efficiency of CH(NH₂)₂Pb_{1âˆ’xâˆ’y}Sn_xâ–¡_yBr₃. Journal of Materials Chemistry C, 2020, 8, 10362-10368.	2.7	13
39	Exploring N-Rich Phases in Li_{<i>x</i>}N_{<i>y</i>} Clusters for Hydrogen Storage at Nanoscale. Journal of Physical Chemistry Letters, 2015, 6, 3726-3730.	2.1	12
40	Insights into enhanced stability and activity of silica modified SiC supported iron oxide catalyst in sulfuric acid decomposition. Applied Catalysis B: Environmental, 2021, 284, 119613.	10.8	12
41	Theoretical insights to excitonic effect in lead bromide perovskites. Applied Physics Letters, 2021, 118, .	1.5	12
42	Ferrocene-derived Fe-metalated porous organic polymer for the core planarity-triggered detoxification of chemical warfare agents. Chemical Communications, 2022, 58, 7789-7792.	2.2	12
43	Dehydrogenation Mechanism of Monoammoniated Lithium Amidoborane [Li(NH3)NH2BH3]. Journal of Physical Chemistry C, 2012, 116, 8859-8864.	1.5	11
44	Origin of Rashba Spin Splitting and Strain Tunability in Ferroelectric Bulk CsPbF₃. Journal of Physical Chemistry Letters, 2021, 12, 9539-9546.	2.1	10
45	Rashba spin splitting and anomalous spin textures in the bulk ferroelectric oxide perovskite KIO₃. Materials Advances, 2022, 3, 4170-4178.	2.6	10
46	A first-principles study of the IIIâ€“IVâ€“V semiconductor nanosheets. Physical Chemistry Chemical Physics, 2015, 17, 1039-1046.	1.3	9
47	Elucidating the Role of Temperature and Pressure to the Thermodynamic Stability of Charged Defects in Complex Metal-Hydrides: A Case Study of NaAlH4. Journal of Physical Chemistry C, 2019, 123, 62-69.	1.5	9
48	Sublattice mixing in Cs2AgInCl6 for enhanced optical properties from first-principles. Applied Physics Letters, 2021, 118, .	1.5	9
49	Chalcogenide Perovskites (ABS₃; A = Ba, Ca, Sr; B = Hf, Sn): An Emerging Class of Semiconductors for Optoelectronics. Journal of Physical Chemistry Letters, 2022, 13, 6439-6446.	2.1	9
50	Micro-structural origin of elongation in swift heavy ion irradiated Ni nanoparticles: A combined EXAFS and DFT study. Acta Materialia, 2016, 121, 37-45.	3.8	8
51	Structure and Electronic Properties of Transition-Metal/Mg Bimetallic Clusters at Realistic Temperatures and Oxygen Partial Pressures. Journal of Physical Chemistry C, 2018, 122, 16788-16794.	1.5	8
52	Importance of Many-Body Dispersion in the Stability of Vacancies and Antisites in Free-Standing Monolayer of MoS₂ from First-Principles Approaches. Journal of Physical Chemistry C, 2020, 124, 1390-1397.	1.5	8
53	Theoretical insights of codoping to modulate electronic structure of $$hbox {TiO}_2$$ and $$hbox {SrTiO}_3$$ for enhanced photocatalytic efficiency. Scientific Reports, 2020, 10, 15372.	1.6	8
54	Capturing excitonic and polaronic effects in lead iodide perovskites using many-body perturbation theory. Journal of Materials Chemistry C, 2021, 9, 17113-17123.	2.7	8

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55	Triggering of spin-flipping-modulated exchange bias in FeCo nanoparticles by electronic excitation. Scientific Reports, 2016, 6, 39292.	1.6	7
56	Exploring Exciton and Polaron Dominated Photophysical Phenomena in Ruddlesdenâ€“Popper Phases of Ba_{<i>n</i>+1}Zr_{<i>n</i>}S_{3<i>n</i>+1} (<i>n</i> = 1â€“3) from Many Body Perturbation Theory. Journal of Physical Chemistry Letters, 2021, 12, 6698-6706.	2.1	7
57	Understanding the Ionic Diffusivity in the (Meta)Stable (Un)doped Solid-State Electrolyte from First-Principles: A Case Study of LISICON. Journal of Physical Chemistry C, 2020, 124, 17485-17493.	1.5	6
58	Unravelling the reactivity of metastable molybdenum carbide nanoclusters in the Câ€“H bond activation of methane, ethane and ethylene. Nanoscale, 2021, 13, 4451-4466.	2.8	6
59	Theoretical insights into Câ€“H bond activation of methane by transition metal clusters: the role of anharmonic effects. Nanoscale Advances, 2021, 3, 575-583.	2.2	6
60	Atomic, electronic, and magnetic properties of bimetallic ZrCo clusters: A first-principles study. Journal of Applied Physics, 2016, 120, .	1.1	5
61	Lead-Free Alloyed Double Perovskites: An Emerging Class of Materials for Optoelectronic Applications. Journal of Physical Chemistry C, 2022, 126, 6753-6760.	1.5	5
62	Unraveling Thermodynamic Stability, Catalytic Activity, and Electronic Structure of [TMxMgyOz]+/0/â€“ Clusters at Realistic Conditions: A Hybrid DFT and ab Initio Thermodynamics Study. Journal of Physical Chemistry C, 2019, 123, 15495-15502.	1.5	4
63	Structure-Dependent (Non)Linear Optical Excitons in Primary Cyclic Ammonium (CnH2nâ€“1NH2; n =) Tj ETQq1 1 0.784314 rgBT /Ov 6821-6831.	1.5	4
64	3d Transition metal decorated B-C-N composite nanostructures for efficient hydrogen storage: A first-principles study. Bulletin of Materials Science, 2009, 32, 353-360.	0.8	3
65	Evidence of local structural influence on the shape driven magnetic anisotropy in electronically excited Ni nanoparticles embedded in SiO2 matrix. Scientific Reports, 2018, 8, 1040.	1.6	3
66	Regeneration of Catalytic Activity of CuOâ€“Cu₂O/In₂O₃ Nanocomposite towards Electrochemical Reduction of CO₂ by UV Light Treatment. Journal of the Electrochemical Society, 2021, 168, 066518.	1.3	2
67	Metastability triggered reactivity in clusters at realistic conditions: a case study of N-doped (TiO₂)_n for photocatalysis. JPhys Materials, 2020, 4, 015001.	1.8	2
68	SO₃ decomposition over silica-modified Î²-SiC supported CuFe₂O₄ catalyst: characterization, performance, and atomistic insights. Nanoscale, 2022, 14, 6876-6887.	2.8	2
69	Electronic, magnetic and optical properties of C, N-doped TiO2 anatase: A hybrid density functional study. AIP Conference Proceedings, 2019, , .	0.3	0
70	Electronic structure and thermodynamic stability of ternary clusters (Ni1Mg1Ox). AIP Conference Proceedings, 2019, , .	0.3	0
71	Thermodynamic stability and electronic structure of bimetallic clusters (TMxMgyOz). Materials Today: Proceedings, 2020, 26, 134-137.	0.9	0
72	Ab-initio study on opto-electronic properties of non-metal doped TiO2. Materials Today: Proceedings, 2020, 26, 94-96.	0.9	0