Saswata Bhattacharya

List of Publications by Citations

64 papers	1,274 citations	18 h-index	34 g-index
73 ext. papers	1,619 ext. citations	5.4 avg, IF	4.92 L-index

#	Paper	IF	Citations
64	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
63	Transition-Metal Decoration Enhanced Room-Temperature Hydrogen Storage in a Defect-Modulated Graphene Sheet. *Journal of Physical Chemistry C*, **2010**, 114, 10297-10301	3.8	120
62	Stability and metastability of clusters in a reactive atmosphere: theoretical evidence for unexpected stoichiometries of MgMOx. *Physical Review Letters*, **2013**, 111, 135501	7.4	62
61	Band Gap Engineering in Cs(NaAg)BiCl Double Perovskite Nanocrystals. *Journal of Physical Chemistry Letters*, **2019**, 10, 5173-5181	6.4	59
60	GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. *Journal of Chemical Theory and Computation*, **2018**, 14, 2246-2264	6.4	51
59	Hydrogen Storage in Ti-Decorated BC4N Nanotube. *Journal of Physical Chemistry C*, **2008**, 112, 17487-17491	3.8	36
58	Efficientab initioschemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. *New Journal of Physics*, **2014**, 16, 123016	2.9	33
57	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	3.8	31
56	Exploring semiconductor substrates for silicene epitaxy. *Applied Physics Letters*, **2013**, 103, 123113	3.4	31
55	A fast and effective approach for reversible wetting-dewetting transitions on ZnO nanowires. *Scientific Reports*, **2016**, 6, 35073	4.9	29
54	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	13	27
53	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	3.8	26
52	Formation of Water Chains on CaO(001): What Drives the 1D Growth?. *Journal of Physical Chemistry Letters*, **2015**, 6, 1204-8	6.4	25
51	Ti-Decorated BC4N Sheet: A planar Nanostructure for High-Capacity Hydrogen Storage. *Journal of Physical Chemistry C*, **2009**, 113, 15783-15787	3.8	25
50	Computational design of nanoclusters by property-based genetic algorithms: Tuning the electronic properties of (TiO2)n clusters. *Physical Review B*, **2015**, 91,	3.3	22
49	Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. *Physical Review Materials*, **2017**, 1,	3.2	21
48	Lithium calcium imide [Li2Ca(NH)2] for hydrogen storage: structural and thermodynamic properties. *Journal of Physical Chemistry B*, **2008**, 112, 11381-4	3.4	20

47	Enhanced Photocurrent Owing to Shuttling of Charge Carriers across 4-Aminothiophenol-Functionalized MoSe-CsPbBr Nanohybrids. *ACS Applied Materials & Interfaces*, **2020**, 12, 7317-7325	9.5	19
46	Unraveling the role of vacancies in the potentially promising thermoelectric clathrates Ba8ZnxGe46□y?y. *Physical Review B*, **2016**, 94,	3.3	18
45	Role of Defects in Photocatalytic Water Splitting: Monodoped vs Codoped SrTiO3. *Journal of Physical Chemistry C*, **2020**, 124, 10272-10279	3.8	16
44	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	7.1	16
43	Reducing lead toxicity in the methylammonium lead halide MAPbI3: Why Sn substitution should be preferred to Pb vacancy for optimum solar cell efficiency. *Physical Review B*, **2020**, 101,	3.3	15
42	Selective electrochemical reduction of CO2 to CO on CuO/In2O3 nanocomposites: role of oxygen vacancies. *Catalysis Science and Technology*, **2019**, 9, 5339-5349	5.5	14
41	Lead-Free Alloyed Double-Perovskite Nanocrystals of Cs2(NaxAg1□x)BiBr6 with Tunable Band Gap. *Journal of Physical Chemistry C*, **2021**, 125, 1954-1962	3.8	13
40	Engineering Electronic Structure and Lattice Dynamics to Achieve Enhanced Thermoelectric Performance of Mn□b Co-Doped GeTe. *Chemistry of Materials*, **2021**, 33, 3611-3620	9.6	12
39	Understanding the efficient electrocatalytic activities of MoSe2□u2S nanoheterostructures. *Journal of Materials Chemistry A*, **2021**, 9, 9837-9848	13	12
38	Dehydrogenation Mechanism of Monoammoniated Lithium Amidoborane [Li(NH3)NH2BH3]. *Journal of Physical Chemistry C*, **2012**, 116, 8859-8864	3.8	11
37	Metal-organic frameworks functionalized smart textiles for adsorptive removal of hazardous aromatic pollutants from ambient air. *Journal of Hazardous Materials*, **2021**, 411, 125056	12.8	11
36	Stability of non-metal dopants to tune the photo-absorption of TiO at realistic temperatures and oxygen partial pressures: A hybrid DFT study. *Scientific Reports*, **2019**, 9, 11427	4.9	10
35	Exploring N-Rich Phases in Li(x)N(y) Clusters for Hydrogen Storage at Nanoscale. *Journal of Physical Chemistry Letters*, **2015**, 6, 3726-30	6.4	10
34	Innovative Approach to Photo-Chemiresistive Sensing Technology: Surface-Fluorinated SnO for VOC Detection. *ACS Applied Materials & Interfaces*, **2020**, 12, 37320-37329	9.5	10
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	3.6	9
32	Unraveling The Origin of Enhanced Field Emission from Irradiated FeCo-SiO2 Nanocomposites: A Combined Experimental and First-Principles Based Study. *ACS Applied Materials & Interfaces*, **2016**, 8, 4994-5001	9.5	9
31	A first-principles study of the III-IV-V semiconductor nanosheets. *Physical Chemistry Chemical Physics*, **2015**, 17, 1039-46	3.6	7
30	Theoretical insights of codoping to modulate electronic structure of [Formula: see text] and [Formula: see text] for enhanced photocatalytic efficiency. *Scientific Reports*, **2020**, 10, 15372	4.9	7

29	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	3.8	7
28	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	3.8	7
27	Micro-structural origin of elongation in swift heavy ion irradiated Ni nanoparticles: A combined EXAFS and DFT study. *Acta Materialia*, **2016**, 121, 37-45	8.4	6
26	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	9.5	6
25	Triggering of spin-flipping-modulated exchange bias in FeCo nanoparticles by electronic excitation. *Scientific Reports*, **2016**, 6, 39292	4.9	6
24	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	3.8	5
23	High-throughput screening to modulate electronic and optical properties of alloyed Cs2AgBiCl6 for enhanced solar cell efficiency. *JPhys Materials*, **2021**, 4, 025005	4.2	5
22	MoS2 and Janus (MoSSe) based 2D van der Waals heterostructures: emerging direct Z-scheme photocatalysts. *Nanoscale Advances*, **2021**, 3, 2837-2845	5.1	5
21	Unraveling Thermodynamic Stability, Catalytic Activity, and Electronic Structure of [TMxMgyOz]+/0/□Clusters at Realistic Conditions: A Hybrid DFT and ab Initio Thermodynamics Study. *Journal of Physical Chemistry C*, **2019**, 123, 15495-15502	3.8	4
20	Understanding the role of Sn substitution and Pb-? in enhancing the optical properties and solar cell efficiency of CH(NH2)2Pb1-□-ySnx?yBr3. *Journal of Materials Chemistry C*, **2020**, 8, 10362-10368	7.1	4
19	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	3.8	4
18	Optoelectronic Properties of Chalcogenide Perovskites by Many-Body Perturbation Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 5301-5307	6.4	4
17	Atomic, electronic, and magnetic properties of bimetallic ZrCo clusters: A first-principles study. *Journal of Applied Physics*, **2016**, 120, 094301	2.5	4
16	Unravelling the reactivity of metastable molybdenum carbide nanoclusters in the C-H bond activation of methane, ethane and ethylene. *Nanoscale*, **2021**, 13, 4451-4466	7.7	4
15	Sublattice mixing in Cs2AgInCl6 for enhanced optical properties from first-principles. *Applied Physics Letters*, **2021**, 118, 021901	3.4	4
14	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	1.7	3
13	Theoretical insights to excitonic effect in lead bromide perovskites. *Applied Physics Letters*, **2021**, 118, 192103	3.4	3
12	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	21.8	3

11	Theoretical insights into C□H bond activation of methane by transition metal clusters: the role of anharmonic effects. *Nanoscale Advances*, **2021**, 3, 575-583	5.1	3
10	Metastability triggered reactivity in clusters at realistic conditions: a case study of N-doped (TiO2) n for photocatalysis. *JPhys Materials*, **2020**, 4, 015001	4.2	2
9	Elucidating the origin of magnetic ordering in ferroelectric BaTiO d thin film via electronic structure modification. *Journal of Physics Condensed Matter*, **2019**, 31, 205001	1.8	2
8	Origin of Rashba Spin Splitting and Strain Tunability in Ferroelectric Bulk CsPbF. *Journal of Physical Chemistry Letters*, **2021**, 12, 9539-9546	6.4	2
7	Evidence of local structural influence on the shape driven magnetic anisotropy in electronically excited Ni nanoparticles embedded in SiO matrix. *Scientific Reports*, **2018**, 8, 1040	4.9	1
6	Structure-Dependent (Non)Linear Optical Excitons in Primary Cyclic Ammonium (CnH2n□NH2; n = 3□8)-Based Inorganic□Organic Hybrid Semiconductor Series. *Journal of Physical Chemistry C*, **2021**, 125, 6821-6831	3.8	1
5	Regeneration of Catalytic Activity of CuO□Cu2O/In2O3 Nanocomposite towards Electrochemical Reduction of CO2 by UV Light Treatment. *Journal of the Electrochemical Society*, **2021**, 168, 066518	3.9	1
4	Exploring Exciton and Polaron Dominated Photophysical Phenomena in Ruddlesden-Popper Phases of BaZrS (= 1-3) from Many Body Perturbation Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 6698-6706	6.4	1
3	Ferrocene Derived Fe-Metalated Porous-Organic-Polymer for Core Planarity Triggered Detoxification of Chemical Warfare Agents. *Chemical Communications*,	5.8	1
2	Thermodynamic stability and electronic structure of bimetallic clusters (TMxMgyOz). *Materials Today: Proceedings*, **2020**, 26, 134-137	1.4	
1	Ab-initio study on opto-electronic properties of non-metal doped TiO2. *Materials Today: Proceedings*, **2020**, 26, 94-96	1.4	