# Saswata Bhattacharya

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 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 | 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 |
| 63 | Structure-Dependent (Non)Linear Optical Excitons in Primary Cyclic Ammonium (CnH2n+1NH2; n = 3−8)-Based Inorganic−Organic Hybrid Semiconductor Series. *Journal of Physical Chemistry C*, **2021**, 125, 6821-6831 | 3.8 | 1 |
| 62 | Theoretical insights to excitonic effect in lead bromide perovskites. *Applied Physics Letters*, **2021**, 118, 192103 | 3.4 | 3 |
| 61 | Engineering Electronic Structure and Lattice Dynamics to Achieve Enhanced Thermoelectric Performance of MnSb Co-Doped GeTe. *Chemistry of Materials*, **2021**, 33, 3611-3620 | 9.6 | 12 |
| 60 | 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 |
| 59 | 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 |
| 58 | Optoelectronic Properties of Chalcogenide Perovskites by Many-Body Perturbation Theory. *Journal of Physical Chemistry Letters*, **2021**, 12, 5301-5307 | 6.4 | 4 |
| 57 | 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 |
| 56 | 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 |
| 55 | 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 |
| 54 | Sublattice mixing in Cs2AgInCl6 for enhanced optical properties from first-principles. *Applied Physics Letters*, **2021**, 118, 021901 | 3.4 | 4 |
| 53 | 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 |
| 52 | MoS2 and Janus (MoSSe) based 2D van der Waals heterostructures: emerging direct Z-scheme photocatalysts. *Nanoscale Advances*, **2021**, 3, 2837-2845 | 5.1 | 5 |
| 51 | Origin of Rashba Spin Splitting and Strain Tunability in Ferroelectric Bulk CsPbF. *Journal of Physical Chemistry Letters*, **2021**, 12, 9539-9546 | 6.4 | 2 |
| 50 | Understanding the efficient electrocatalytic activities of MoSe2−Cu2S nanoheterostructures. *Journal of Materials Chemistry A*, **2021**, 9, 9837-9848 | 13 | 12 |
| 49 | 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 |
| 48 | 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 |

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| 47 | 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 |
| 46 | 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 |
| 45 | 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 |
| 44 | Role of Defects in Photocatalytic Water Splitting: Monodoped vs Codoped SrTiO3. *Journal of Physical Chemistry C*, **2020**, 124, 10272-10279 | 3.8 | 16 |
| 43 | 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 |
| 42 | 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 |
| 41 | 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 |
| 40 | 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 |
| 39 | Innovative Approach to Photo-Chemiresistive Sensing Technology: Surface-Fluorinated SnO for VOC Detection. *ACS Applied Materials & Interfaces*, **2020**, 12, 37320-37329 | 9.5 | 10 |
| 38 | 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 |
| 37 | Thermodynamic stability and electronic structure of bimetallic clusters (TMxMgyOz). *Materials Today: Proceedings*, **2020**, 26, 134-137 | 1.4 | |
| 36 | Ab-initio study on opto-electronic properties of non-metal doped TiO2. *Materials Today: Proceedings*, **2020**, 26, 94-96 | 1.4 | |
| 35 | 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 |
| 34 | 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 |
| 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 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 |
| 31 | Band Gap Engineering in Cs(NaAg)BiCl Double Perovskite Nanocrystals. *Journal of Physical Chemistry Letters*, **2019**, 10, 5173-5181 | 6.4 | 59 |
| 30 | 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 |

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| 29 | 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 |
| 28 | 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 |
| 27 | GAtor: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction. *Journal of Chemical Theory and Computation*, **2018**, 14, 2246-2264 | 6.4 | 51 |
| 26 | 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 |
| 25 | 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 |
| 24 | Theoretical evidence for unexpected O-rich phases at corners of MgO surfaces. *Physical Review Materials*, **2017**, 1, | 3.2 | 21 |
| 23 | 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 |
| 22 | Unraveling the role of vacancies in the potentially promising thermoelectric clathrates Ba8ZnxGe46□?y. *Physical Review B*, **2016**, 94, | 3.3 | 18 |
| 21 | 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 |
| 20 | 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 |
| 19 | A fast and effective approach for reversible wetting-dewetting transitions on ZnO nanowires. *Scientific Reports*, **2016**, 6, 35073 | 4.9 | 29 |
| 18 | Triggering of spin-flipping-modulated exchange bias in FeCo nanoparticles by electronic excitation. *Scientific Reports*, **2016**, 6, 39292 | 4.9 | 6 |
| 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 | 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 |
| 15 | Formation of Water Chains on CaO(001): What Drives the 1D Growth?. *Journal of Physical Chemistry Letters*, **2015**, 6, 1204-8 | 6.4 | 25 |
| 14 | 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 |
| 13 | 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 |
| 12 | A first-principles study of the III-IV-V semiconductor nanosheets. *Physical Chemistry Chemical Physics*, **2015**, 17, 1039-46 | 3.6 | 7 |

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| 11 | 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 |
| 10 | 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 |
| 9 | Exploring semiconductor substrates for silicene epitaxy. *Applied Physics Letters*, **2013**, 103, 123113 | 3.4 | 31 |
| 8 | Dehydrogenation Mechanism of Monoammoniated Lithium Amidoborane [Li(NH3)NH2BH3]. *Journal of Physical Chemistry C*, **2012**, 116, 8859-8864 | 3.8 | 11 |
| 7 | 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 |
| 6 | 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 |
| 5 | 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 |
| 4 | Ti-Decorated BC4N Sheet: A planar Nanostructure for High-Capacity Hydrogen Storage. *Journal of Physical Chemistry C*, **2009**, 113, 15783-15787 | 3.8 | 25 |
| 3 | Hydrogen Storage in Ti-Decorated BC4N Nanotube. *Journal of Physical Chemistry C*, **2008**, 112, 17487-17491 | 3.8 | 36 |
| 2 | 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 |
| 1 | Ferrocene Derived Fe-Metalated Porous-Organic-Polymer for Core Planarity Triggered Detoxification of Chemical Warfare Agents. *Chemical Communications*, | 5.8 | 1 |