



Bikram Kumar Das

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Summary of CV

This section describes briefly a summary of your career in science, academic and research; the main scientific and technological achievements and goals in your line of research in the medium -and long- term. It also includes other important aspects or peculiarities.

My research career is driven by the ambition to harness advanced materials simulation techniques such as Density Functional Theory (DFT), ab initio Molecular Dynamics (AIMD), Classical MD (CMD), and Machine Learning to address challenges in materials science. I specialize in developing computational methodologies that provide mechanistic insights and actionable design rules, with a current focus on designing efficient and cost-effective solid state batteries.

To date, my work has led to 40 publications in Q1/D1 (40/27) journals (6 as first author), with 989 citations and an h-index of 17 (Scopus/Google Scholar). I regularly review articles for journals such as 2D Mater., Energy Storage Mater., Adv. Func. Mater. etc. My expertise spans DFT, AIMD, CMD, and simulation packages (VASP, CASTEP, LAMMPS, CHGNET), complemented by strong programming skills. Beyond technical strengths, I am committed to leading projects independently and collaboratively within interdisciplinary teams.

I was educated in India, obtaining a B.Sc. (2012) and M.Sc. (2014) in Physics, followed by a Ph.D. in Science (2022) at Jadavpur University, Kolkata. Funded by a DST-INSPIRE Fellowship, my doctoral work with Prof. KK Chattopadhyay involved ab-initio investigations of doped/adsorbed graphyne, graphdiyne, and related 2D systems for energy applications. Collaborations broadened my scope into simulations of photocatalysis, conductivity and cluster expansion. During my Ph.D., I received two international travel grants (DST-SERB and ICTP), presenting research at DIPC (Spain) and ICTP (Italy).

I joined BCAM in April, 2022 as a research technician in the Modeling and Simulation in Life and Materials Sciences (MSLMS) group led by Prof. Elena Akhmatskaya. I became a BCAM Postdoctoral Fellow in Jan., 2023. In 2024 I was awarded the prestigious Juan de la Cierva Postdoctoral Fellowship.

At BCAM, I contribute to three nationally funded projects, CICE21, ICME-2023 and PID2022-136585NB-C22 coordinated by Prof. Akhmatskaya and Dr. M. Bonilla, focusing on (i) SEI formation and evolution chemistry in Li-ion batteries, (ii) the role of adatoms/impurities in hydrogen embedding in steel and (iii) development and application of enhanced simulation techniques for solid state modeling. These projects integrate DFT, AIMD, CMD, and hybrid Monte Carlo methods, in collaboration with the group's partners such as CIC energiGUNE (Spain), Shanghai Key Laboratory (China), CIDEMAT (Colombia) etc. From this work, I have published two high-impact first-author papers (another in preparation) and four collaborative articles. Since September, 2025, I am also supervising an internship project in BCAM.

My current goal is to advance computational methodologies for solid-state batteries while continuing collaboration with Prof. Akhmatskaya, her group, and BCAM's partners. This environment will strongly foster my development as an independent researcher in computational materials science and energy storage.

General quality indicators of scientific research

This section describes briefly the main quality indicators of scientific production (periods of research activity, experience in supervising doctoral theses, total citations, articles in journals of the first quartile, H index...). It also includes other important aspects or peculiarities.

I, Bikram Kumar Das, have completed my doctoral research work at the Department of Physics, Jadavpur University, Kolkata, India under the supervision of Prof. Kalyan Kumar Chattopadhyay. I obtained my Ph.D. degree on July 18th, 2022. Currently, I am working as a Post-doctoral fellow in the research line “Modelling and Simulation in Life and Material Sciences” under the supervision of Prof. Elena Akhmatskaya and Dr. Mauricio R. Bonilla at the Basque Center for Applied Mathematics-BCAM.

Current research interests: (1) development of efficient halide-based solid electrolytes for all-solid-state lithium batteries based on combined DFT, MD and ML (2) SEI formation chemistry in lithium ion batteries. (3) Combined density functional theory and kinetic Monte-Carlo study of - Diffusion of atomic hydrogen in high strength steels and the effect of adatoms/ impurities towards hydrogen embrittlement. (4) development and application of enhanced simulation techniques for solid state modelling.

Research experience:

Density Functional Theory based study of:

- Formation of solid electrolyte interface components in the lithium ion batteries.
- Diffusion of atomic hydrogen in steel alloys.
- Electronic and electrocatalytic activities of Graphynes, Graphdiyne and analogous two dimensional carbon materials.
- Electronic, photocatalytic, thermal properties of various synthesized nanomaterials and their applications.
- Electronic and electrocatalytic properties of two dimensional binary monolayers and transition metal di-chalcogenides.

Ab-initio molecular dynamics study of:

- Decomposition of electrolyte components such as di-methyl carbonate and ethylene carbonate on graphite anode and the formation of SEI components.
- Diffusion kinetics of hydrogen within steel alloys and crack formation.

Skills/Experience:



- Leading density functional theory based codes/packages: VASP, Quantum Espresso and CASTEP.
- classical MD packages: LAMMPS, ReaxFF
- ML-MD packages: CHGNet.
- “Free Energy” method for studying surface reactions
- Ab Initio (DFT based) Molecular Dynamics (MD)
- classical MD
- ML-MD
- Study of thermal transport properties
- Building and maintaining high performance parallel computing clusters.
- Comfortable working in group settings. Have extensive experiences in collaborating with experimentalists in diverse fields.



Bikram Kumar Das

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Current professional situation

Employing entity: ASOC BCAM - BASQUE CENTER FOR APPLIED MATHEMATICS

Professional category: Juan de la Cierva Postdoctoral Fellow

Start date: 01/01/2024

Type of contract: Grant-assisted student (pre or post-doctoral, others) **Dedication regime:** Full time

Identify key words: Density functional theory; Molecular dynamic; Chemistry of solid state; Fuel batteries

Previous positions and activities

	Employing entity	Professional category	Start date
1	ASOC BCAM - BASQUE CENTER FOR APPLIED MATHEMATICS	Postdoctoral Researcher	01/02/2023
2	Researcher Basque Center for Applied Mathematics: BCAM	Research Technician in the Employment category of Researcher	01/04/2022

1 Employing entity: ASOC BCAM - BASQUE CENTER FOR APPLIED MATHEMATICS

Professional category: Postdoctoral Researcher

Start-End date: 01/02/2023 - 31/12/2023



- 2** **Employing entity:** Researcher Basque Center for Applied Mathematics: BCAM **Type of entity:** Public Research Body
Professional category: Research Technician in the Employment category of Researcher
Start-End date: 01/04/2022 - 31/01/2023 **Duration:** 10 months

Summary of professional activity

I am a computational materials scientist with over eight years of research experience spanning PhD and postdoctoral stages. My career has been driven by the ambition to apply and advance first-principles simulations and multiscale modeling to address critical challenges in energy storage and structural materials. During my PhD at Jadavpur University (India), I pioneered the study of doped and adsorbed graphyne/graphdiyne systems, publishing four first-author papers and collaborating with experimentalists in catalysis, alloys, and optoelectronics.

Since 2022, I have been working at the BCAM, Spain, first as a research technician, then as a postdoctoral researcher, and currently as a Juan de la Cierva fellow. At BCAM, I have contributed to multiple nationally funded projects (CICE21/23, ICME-2022/23, PID2022-136585NB-C22) led by Prof. Elena Akhmatkaya and Dr. Mauricio Bonilla. My main contributions include: (i) atomistic studies of SEI formation and evolution in Li-ion batteries using DFT, AIMD, CI-NEB, and reactive force-field MD; (ii) investigations of hydrogen embrittlement in steels, focusing on the role of alloying elements, impurities, and magnetic ordering; and (iii) the development and application of enhanced simulation methodologies for solid-state systems. This research has resulted in high-impact first-author publications, multiple collaborative works. I have also gained initial supervisory experience by mentoring an internship project on solid-state battery.



Education

University education

1st and 2nd cycle studies and pre-Bologna degrees

1 University degree: Doctorate

Name of qualification: Doctor of Philosophy: Science

Degree awarding entity: Jadavpur University,
Kolkata, India

Type of entity: University

Date of qualification: 18/07/2022

2 University degree: Post-graduate

Name of qualification: Mater of Science (Physics)

Degree awarding entity: Jadavpur University,
Kolkata, India

Type of entity: University

Date of qualification: 11/08/2014

3 University degree: Graduate

Name of qualification: Bachelor of Science (Physics Honours)

Degree awarding entity: Jadavpur University,
Kolkata, India

Type of entity: University

Date of qualification: 20/06/2012

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
Spanish	A1	A1	A1	A1	A1
Bengali	C2	C2	C2	C2	C2
English	C2	C2	C2	C2	C2

Scientific and technological activities

Scientific production

H index: 17

Date of application: 25/09/2025

Source of H-Index: GOOGLE SCHOLAR

Publications, scientific and technical documents

- 1** Bikram Kumar Das; Henry A Cort{\'e}s; Mauricio Rinc{\'o}n Bonilla; Menghao Yang; Javier Carrasco; Elena Akhmatskaya. DMC matters: the role of dimethyl carbonate in SEI formation on oxygen functionalized anodes. Journal of Materials Chemistry A. Royal Society of Chemistry, 2025.
Type of production: Scientific paper **Format:** Journal
- 2** Kausik Sardar; Souvik Bhattacharjee; Nripen Besra; Nilesh Mazumder; Bikram Kumar Das; Gautam Majumdar; Kalyan Kumar Chattopadhyay. Dynamic counteraction of Maxwell--Wagner polarization with frequency-dispersive pseudo-inductive effect in V2O5 nanorods: role of oxygen vacancy and detrapped carriers towards RF decoupler. Journal of Physics D: Applied Physics. 58 - 21, pp. 215105 - 215105. IOP Publishing, 2025.
Type of production: Scientific paper **Format:** Journal
- 3** Nabanita Sen; Anup Debnath; Souvik Bhattacharjee; Bikram Kumar Das; Manas Thakur; Arnab Kumar Saha; Kalyan Kumar Chattopadhyay. Efficient Light to Heat Conversion in Sb2Se3 Nanorods and the Role of Macro-channel Imprinted Sb2Se3 Loaded Hybrid Membrane for Superior Desalination Performance. Small. 21 - 7, pp. 2408293 - 2408293. Wiley Online Library, 2025.
Type of production: Scientific paper **Format:** Journal
- 4** H{\'e}ctor D Agudelo; Ferley A Vasquez; Jorge A Calder{\'o}n; Roberto M Torresi; Eduardo Carmine; Bikram Kumar Das; Henry Andr{\'e}s Cort{\'e}s; Mauricio R Bonilla; Elena Akhmatskaya. Enhanced Stability of Spinel LiMn1.5Ni0.5O4 with V Doping for High-Voltage Li-Ion Batteries in Organic and Ionic Liquid Electrolytes. Journal of Alloys and Compounds. pp. 183060 - 183060. Elsevier, 2025.
Type of production: Scientific paper **Format:** Journal
- 5** Suvankar Poddar; Suvankar Mondal; Souvik Bhattacharjee; Pranab Kumar Sarkar; Bikram Kumar Das; Kalyan Kumar Chattopadhyay. Revealing the Effect of Substantial A Site Cation Multiplicity in Lead-Free Double Perovskites for Memristor-Based Synaptic Devices. ACS Applied Materials & Interfaces. 17 - 20, pp. 29884 - 29900. ACS Publications, 2025.
Type of production: Scientific paper **Format:** Journal
- 6** Suvankar Mondal; Soumen Maiti; Tufan Paul; Suvankar Poddar; Bikram Kumar Das; Kalyan Kumar Chattopadhyay. CsPbI3--PVDF composite-based multimode hybrid piezo-triboelectric nanogenerator: self-powered moisture monitoring system. ACS Applied Materials & Interfaces. 16 - 7, pp. 9231 - 9246. ACS Publications, 2024.
Type of production: Scientific paper **Format:** Journal
- 7** Bikram Kumar Das; Poulami Chakraborty; Mingyuan Lu; Mauricio Rinc{\'o}n Bonilla; Elena Akhmatskaya. The impact of Mn and Al on the trapping and diffusion of hydrogen in γ -Fe: An atomistic insight. International Journal of Hydrogen Energy. 83, pp. 731 - 744. Elsevier, 2024.
Type of production: Scientific paper **Format:** Journal

- 8** Arnab Das; Bikram Kumar Das; KK Chattopadhyay. Coinage metals doped 1T' WS₂ as efficient bifunctional electrocatalyst towards ORR and HER: a first principles study. Computational Materials Science. 229, pp. 112418 - 112418. Elsevier, 2023.
Type of production: Scientific paper **Format:** Journal
- 9** Ankita Chandra; Shrabani Ghosh; Bikram Kumar Das; Suvra Pal; Supratim Maity; Biswajit Das; Sourav Sarkar; KK Chattopadhyay. Experimental and theoretical approaches of electron emission from hydrophobic rGO modified silicon nanowires. Applied Surface Science. 608, pp. 155174 - 155174. Elsevier, 2023.
Type of production: Scientific paper **Format:** Journal
- 10** Bikram Kumar Das; Anibrata Banerjee; Arnab Das; Kalyan Kumar Chattopadhyay. Graphyne supported Co₁₃, Fe₁₃ and Ni₁₃ nano-cluster as efficient electrocatalysts for nitrogen reduction reaction: A first principles study. Catalysis Today. 423, pp. 113906 - 113906. Elsevier, 2023.
Type of production: Scientific paper **Format:** Journal
- 11** Dimitra Das; Bikram Kumar Das; Ratna Sarkar; Somnath Mukherjee; Kalyan Kumar Chattopadhyay. Highly exfoliated graphitic carbon nitride for efficient removal of wastewater pollutants: Insights from DFT and statistical modelling. Environmental Research. 221, pp. 115263 - 115263. Elsevier, 2023.
Type of production: Scientific paper **Format:** Journal
- 12** Dipayan Roy; Bikram Kumar Das; S Najes Riaz; Dimitra Das; Sourav Sarkar; Kalyan Kumar Chattopadhyay. Oxygen vacancy-induced band engineering and metal unsaturation in MoS₂--MoO₃ with spillover-based confined catalysis. ACS Applied Energy Materials. 6 - 9, pp. 4892 - 4908. ACS Publications, 2023.
Type of production: Scientific paper **Format:** Journal
- 13** Arnab Das; Dipayan Roy; Bikram Kumar Das; Md Imran Ansari; Kalyan Kumar Chattopadhyay; Sourav Sarkar. Zinc doping induced WS₂ accelerating the HER and ORR kinetics: a theoretical and experimental validation. Catalysis Today. 423, pp. 113921 - 113921. Elsevier, 2023.
Type of production: Scientific paper **Format:** Journal
- 14** Dimitra Das; Bikram Kumar Das; Ratna Sarkar; Somnath Mukherjee; Kalyan Kumar Chattopadhyay. Copper and nickel decorated g-C₃N₄ as superior catalysts for reduction of toxic pollutants: a combined experimental and theoretical approach. Applied Surface Science. 580, pp. 152137 - 152137. Elsevier, 2022.
Type of production: Scientific paper **Format:** Journal
- 15** Brahami Das; Biswajit Das; Nirmayla Sankar Das; Suvra Pal; Bikram Kumar Das; Ratna Sarkar; Rimpa Khan; Subrata Sarkar; Kalyan Kumar Chattopadhyay. Enhanced field emission properties of rGO wrapped Ga₂O₃ micro/nanobricks: Experimental investigation with theoretical validation. Journal of Alloys and Compounds. 902, pp. 163726 - 163726. Elsevier, 2022.
Type of production: Scientific paper **Format:** Journal
- 16** Bikram Kumar Das; Dipayan Sen; KK Chattopadhyay. Mechanism of oxygen reduction reaction in alkaline medium on nitrogen-doped graphyne and graphdiyne families: a first principles study. ChemPhysChem. 23 - 9, pp. e202100900 - e202100900. Wiley Online Library, 2022.
Type of production: Scientific paper **Format:** Journal
- 17** Dipayan Roy; Antika Das; Rajarshi Roy; Dimitra Das; Bikram Kumar Das; Uttam Kumar Ghorai; Kalyan Kumar Chattopadhyay; Sourav Sarkar. Probing the emission dynamics in nitrogen-doped carbon dots by reversible capping with mercury (ii) through surface chemistry. New Journal of Chemistry. 46 - 30, pp. 14690 - 14702. Royal Society of Chemistry, 2022.
Type of production: Scientific paper **Format:** Journal

- 18** Anibrata Banerjee; Bikram Kumar Das; Kalyan Kumar Chattopadhyay. Significant enhancement of lattice thermal conductivity of monolayer AlN under bi-axial strain: a first principles study. *Physical Chemistry Chemical Physics*. 24 - 26, pp. 16065 - 16074. Royal Society of Chemistry, 2022.
Type of production: Scientific paper **Format:** Journal
- 19** Dipayan Roy; Karamjyoti Panigrahi; Bikram Kumar Das; Uday K Ghorui; Souvik Bhattacharjee; Madhupriya Samanta; Sourav Sarkar; Kalyan Kumar Chattopadhyay. Boron vacancy: a strategy to boost the oxygen reduction reaction of hexagonal boron nitride nanosheet in hBN–MoS₂ heterostructure. *Nanoscale Advances*. 3, pp. 4739. 2021.
Type of production: Scientific paper **Format:** Journal
- 20** Nripen Besra; Kausik Sardar; Nilesh Mazumder; Souvik Bhattacharjee; Anjan Das; Bikram Kumar Das; Saikat Sarkar; Kalyan Kumar Chattopadhyay. CH₃NH₃PbI₃ as a radio frequency decoupling capacitor: interplay between Maxwell–Wagner polarization and a pseudo inductive response. *Journal of Physics D: Applied Physics*. 54, pp. 175105. 2021.
Type of production: Scientific paper **Format:** Journal
- 21** Tufan Paul; Soumen Maiti; Biplob Kr Chatterjee; Partha Bairi; Bikram Kumar Das; Subhasish Thakur; Kalyan Kumar Chattopadhyay. Electrochemical Performance of 3D Network CsPbBr₃ Perovskite Anodes for Li-Ion Batteries: Experimental Venture with Theoretical Expedition. *The Journal of Physical Chemistry: C*. 125 - 31, pp. 16892 - 16902. 2021.
Type of production: Scientific paper
- 22** Shrabani Ghosh; Supratim Maity; Ankita Chandra; Bikram Kumar Das; Nripen Besra; Samrat Sarkar; Sourav Sarkar; Kalyan Kumar Chattopadhyay. Enhanced electron emission from ternary solid solution-MWCNT hybrid with theoretical validation. *Materials Science in Semiconductor Processing*. 127, pp. 105674. 2021.
Type of production: Scientific paper **Format:** Journal
- 23** Saikat Sarkar; Rajarshi Roy; Bikram Kumar Das; Kalyan Kumar Chattopadhyay. Temperature-dependent site selection of boron doping in chemically derived graphene. *Carbon*. 184, pp. 253 - 265. 2021.
Type of production: Scientific paper **Format:** Journal
- 24** Tufan Paul; Dimitra Das; Bikram Kumar Das; Saikat Sarkar; Soumen Maiti; Kalyan Kumar Chattopadhyay. CsPbBrCl₂/g-C₃N₄ type II heterojunction as efficient visible range photocatalyst. *Journal of Hazardous Materials*. 380, pp. 120855. 2020.
Type of production: Scientific paper **Format:** Journal
- 25** Ratna Sarkar; Dimitra Das; Bikram Kumar Das; Anuradha Mitra; Nirmalya S Das; Subrata Sarkar; Kalyan Kumar Chattopadhyay. Hollow micro-spherical bismuth oxy-chloride for superior visible light induced dye-sensitized photocatalytic activity and its theoretical insight. *Materials research Bulletin*. 125, pp. 110778. 2020.
Type of production: Scientific paper **Format:** Journal
- 26** Suvankar Mondal; Tufan Paul; Soumen Maiti; Bikram Kumar Das; Kalyan Kumar Chattopadhyay. Human motion interactive mechanical energy harvester based on all inorganic perovskite-PVDF. *Nano Energy*. 74, pp. 104870. 2020.
Type of production: Scientific paper **Format:** Journal
- 27** Supratim Maity; Biswajit Das; Madhupriya Samanta; Bikram Kumar Das; Shrabani Ghosh; Kalyan Kumar Chattopadhyay. MoSe₂-Amorphous CNT Hierarchical Hybrid Core–Shell Structure for Efficient Hydrogen Evolution Reaction. *ACS Applied Energy Materials*. 3 - 5, pp. 5067 - 5076. 2020.
Type of production: Scientific paper **Format:** Journal

- 28** Brahmi Das; Biswajit Das; Nirmayla Sankar Das; Suvra Pal; Bikram Kumar Das; Subrata Sarkar; Kalyan Kumar Chattopadhyay. Novel Ag₂O-Ga₂O₃ type II p-n heterojunction as an efficient water cleanser for green cleaning technology. Applied Surface Science. 515, pp. 145958. 2020.
Type of production: Scientific paper **Format:** Journal
- 29** Dipayan Roy; Saikat Sarkar; Kaustav Bhattacharjee; Karamjyoti Panigrahi; Bikram Kumar Das; Kausik Sardar; Sourav Sarkar; Kalyan Kumar Chattopadhyay. Site specific nitrogen incorporation in reduced graphene oxide using imidazole as a novel reducing agent for efficient oxygen reduction reaction and improved supercapacitive performance. Carbon. 166, pp. 361 - 373. 2020.
Type of production: Scientific paper **Format:** Journal
- 30** Dipanwita Mitra; Promita Howli; Bikram Kumar Das; Nirmalya Sankar Das; Paramita Chattopadhyay; Kalyan Kumar Chattopadhyay. Size and phase dependent thermal conductivity of TiO₂-water nanofluid with theoretical insight. Journal of Molecular Liquids. 302, pp. 112499. 2020.
Type of production: Scientific paper **Format:** Journal
- 31** Dipanwita Mitra; Souvik Bhattacharjee; Nilesh Mazumder; Bikram Kumar Das; Paramita Chattopadhyay; Kalyan Kumar Chattopadhyay. Strain-induced partial phase transition in TiO₂ nanoparticles manifesting frequency dispersive pseudo-inductive switching of capacitance. Ceramics International. 46 - 12, pp. 20437 - 20447. 2020.
Type of production: Scientific paper **Format:** Journal
- 32** Suvra Pal; Nirmalya Sankar Das; Brahmi Das; Bikram Kumar Das; Subhadipta Mukhopadhyay; Kalyan Kumar Chattopadhyay. V doped BaSnO₃ nanocubes as a field emitting material: Experimental and theoretical investigation. Applied surface science. 530, pp. 147102. 2020.
Type of production: Scientific paper **Format:** Journal
- 33** Antika Das; Karamjyoti Panigrahi; Subhajit Saha; Bikram Kumar Das; Nirmalya Sankar Das; Saikat Sarkar; Rituparna Chatterjee; Kalyan Kumar Chattopadhyay. Yellow emitting Fe₃O₄/ZnS hybrid: A probe for in-vitro dermatoglyphics and anti-counterfeiting applications. Materials Research Bulletin. 131, pp. 110966. 2020.
Type of production: Scientific paper **Format:** Journal
- 34** Tufan Paul; Soumen Maiti; Nripen Besra; Biplab Kr Chatterjee; Bikram Kumar Das; Subhasish Thakur; Saikat Sarkar; Nirmalya Sankar Das; Kalyan Kumar Chattopadhyay. Tailored CsPbX₃ Nanorods for Electron-Emission Nanodevices. ACS Applied Nano Materials. 2 - 9, pp. 5942 - 5951. 2019.
Type of production: Scientific paper **Format:** Journal
- 35** Dipayan Sen; Bikram Kumar Das; Subhajit Saha; Rajarshi Roy; Anuradha Mitra; Kalyan Kumar Chattopadhyay. sp³ bonded 2-dimensional allotrope of carbon: A first-principles prediction. Carbon. 146, pp. 430 - 437. 2019.
Type of production: Scientific paper **Format:** Journal
- 36** Tufan Paul; Biplab Chatterjee; Soumen Maity; Saikat Sarkar; Nripen Besra; Bikram Kumar Das; Karamjyoti Panigrahi; Subhasish Thakur; Uttam Kumar Ghorai; Kalyan Kumar Chattopadhyay. Tunable cathodoluminescence over the entire visible window from all-inorganic perovskite CsPbX₃ 1D architecture. Journal of Materials Chemistry C. 6, pp. 3322. 2018.
Type of production: Scientific paper **Format:** Journal
- 37** Shrabani Ghosh; Samrat Sarkar; Bikram Kumar Das; Dipayan Sen; Madhupriya Samanta; Kalyan Kumar Chattopadhyay. Band edge tuned ZnxCd1-xS solid solution nanopowders for efficient solar photocatalysis. Physical Chemistry Chemical physics. 19, pp. 29998 - 30009. 2017.
Type of production: Scientific paper **Format:** Journal



- 38** Nripen Besra; Shreyasi Pal; Bikram Kumar Das; Kalyan Kumar Chattopadhyay. Perovskites beyond photovoltaics: field emission from morphology-tailored nanostructured methylammonium lead triiodide. *Physical Chemistry Chemical physics*. 19, pp. 26708 - 26717. 2017.

Type of production: Scientific paper

Format: Journal

- 39** Bikram Kumar Das; Dipayan Sen; Kalyan Kumar Chattopadhyay. Implications of boron doping on electrocatalytic activities of graphyne and graphdiyne families: a first principles study. *Physical Chemistry Chemical Physics*. 18, pp. 2949 - 2958. 2016.

Type of production: Scientific paper

Format: Journal

- 40** Bikram Kumar Das; Dipayan Sen; Kalyan Kumar Chattopadhyay. Nitrogen doping in acetylene bonded two dimensional carbon crystals: Ab-initio forecast of electrocatalytic activities vis-à-vis boron doping. *Carbon*. 105, pp. 330 - 339. 2016.

Type of production: Scientific paper

Format: Journal

Works submitted to national or international conferences

- 1** **Title of the work:** Talk: DMC matters: the key role of dimethyl carbonate in SEI formation on oxygen functionalized anodes
Name of the conference: 6th edition of the Power our Future conference (POF'25)
City of event: Vitoria-Gasteiz, Spain
Date of event: 2025
Organising entity: CIC EnergiGUNE
- 2** **Title of the work:** Talk: The impact of Mn and Al on the trapping and diffusion of hydrogen in non-magnetic and antiferromagnetic FCC iron: An atomistic insight
Name of the conference: Gordon Research Seminar (GRS) on Hydrogen-Metal Systems
City of event: Les Diablerets, Switzerland
Date of event: 2025
- 3** **Title of the work:** Talk: The impact of Mn and Al on the trapping and diffusion of hydrogen in γ -Fe: An atomistic insight
Name of the conference: DPG Spring Meeting of the Condensed Matter Section 2025
City of event: Regensburg, Germany
Date of event: 2025
Organising entity: University of Regensburg
- 4** **Title of the work:** Talk: The impact of Mn and Al on the trapping and diffusion of hydrogen in γ -Fe: An atomistic insight
Name of the conference: Journées de la Matière Condensée (JMC)
City of event: Marseille, France
Date of event: 2024
Organising entity: Aix-Marseille University
- 5** **Title of the work:** Poster Presentation: Examining the impact of manganese and aluminium on hydrogen diffusion in steel alloys: A first principles approach
Name of the conference: Gordon Research Seminar (GRS) on Hydrogen-Metal Systems
City of event: Les Diablerets, Switzerland
Date of event: 2023



- 6** **Title of the work:** Poster: Pure and B/ N doped Graphdiyne as a nano reactor for ORR, a competitor for Platinum: A first principles study
Name of the conference: 20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods
City of event: Trieste, Italy
Date of event: 2021
Organising entity: International Centre for Theoretical Physics (ICTP)
- 7** **Title of the work:** Poster: Band gap modulation of dynamically stable bilayer and trilayer WS₂ configurations under external electric field
Name of the conference: Computational School on Electronic Excitations in Novel Materials Using the Yambo Code – 2020
City of event: Trieste, Italy
Date of event: 2020
Organising entity: International Center for Theoretical Physics (ICTP)
- 8** **Title of the work:** Poster: Band gap modulation of dynamically stable bilayer and trilayer WS₂ configurations under external electric field
Name of the conference: Workshop on Computational Physics and Materials Science: Total Energy and Force Methods 2020
City of event: San Sebastian, Spain
Date of event: 2020
Organising entity: Donostia International Physics Center (DIPC)
- 9** **Title of the work:** Poster: Mechanism of Oxygen Reduction Reaction in Alkaline Medium on Nitrogen doped Graphyne and Graphdiyne families: A First Principles Study
Name of the conference: International Conference on Nano Science and Technology (ICONSAT) - 2020
City of event: Kolkata, India
Date of event: 2020
Organising entity: S.N. Bose National Centre for Basic Sciences (SNBNCBS)
- 10** **Title of the work:** Poster: Lattice thermal conductivity of monolayer AlN : A first-principles study
Name of the conference: Conference on Nanophononics, Bridging Statistical Physics, Molecular Modeling and Experiments - 2019
City of event: Trieste, Italy
Date of event: 2019
Organising entity: International Center for Theoretical Physics (ICTP)
- 11** **Title of the work:** Poster: Ab-initio forecast of the electrocatalytic activities of Nitrogen doped 2-D acetylene bonded Carbon crystal family vis-à-vis Boron doping
Name of the conference: Asian Consortium on Computational Materials Science - Theme meeting (ACCMS-TM)
City of event: Chennai, India
Date of event: 2016
Organising entity: SRM University, Chennai
- 12** **Title of the work:** Poster: Implications of boron doping on electrocatalytic activities of graphyne and graphdiyne families: a first principles study
Name of the conference: International Conference on Nano Science and Technology (ICONSAT) - 2016
City of event: Pune, India
Date of event: 2016
Organising entity: IISER Pune



Other achievements

Obtained grants and scholarships

- 1** **Name of the grant:** Juan de la Cierva Individual Postdoctoral Fellowship
Awarding entity: Ministerio de Ciencia, Innovación y Universidades and the Agencia Estatal de Investigación, Spain
Conferral date: 01/01/2024 **Duration:** 2 years
End date: 31/12/2025
Entity where activity was carried out: ASOC BCAM - BASQUE CENTER FOR APPLIED MATHEMATICS
- 2** **Name of the grant:** DST-INSPIRE doctoral (PhD) fellowship
Awarding entity: Department of Science & Technology, Govt. of India
Duration: 5 years - 6 months
Entity where activity was carried out: Jadavpur University