

Dr. Abir Bhattacharya

Assistant Professor

Department of Physics

Contact Information

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Specialization

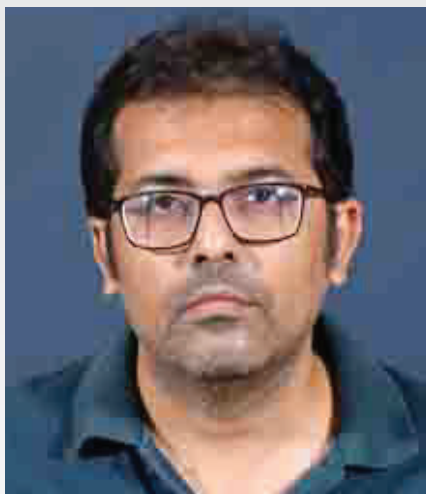
- X-ray Crystallography

Biographical Sketch

Dr. Abir Bhattacharya is currently associated as Assistant Professor (UGC), in the Department of Physics, The Bhawanipur Education Society College, affiliated to University of Calcutta. Prior to joining this institution, he worked as a Assistant Professor and HOD, In the Department of Physics, Amity University Kolkata. He completed his Bachelor and Master degrees from University of Calcutta, Kolkata, with Electronics as Specialization. He Pursued his Ph.D degree of Science from the Department of Physics, Jadavpur University under the supervision of Prof. Alok K. Mukherjee. During his Ph.D he has worked with Lupin pharmaceuticals and has published two papers jointly with them in reputed International Journals. He has teaching experience of 10 years in different undergraduate and post graduate colleges and Universities. He has published numerous research papers in internationally reputed journals. He has also participated in several national and international seminars / webinars / workshops / conferences. He has authored one book chapter till date, which is based on his individual research work. He has guided as well as currently guiding several post graduate students of Amity University Kolkata for their summer projects and final semester major projects. His current research interests are Hirshfeld Surface analysis, X-ray Crystallography, Powder Diffraction, Drug Design, Density Functional Theory etc.



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Academic Qualifications

Jadavpur University and Indian Association for the Cultivation of Science

- Ph.D completed under the supervision of Prof. Alok K. Mukherjee in The Department of Physics, Jadavpur University, May, 2015. Thesis title: "Crystal and molecular structure determination of some organic compounds and metal organic complexes using single -and powder-crystal X-ray diffraction".
- Senior Research Fellow, Department of Physics, Jadavpur University, under Prof. Alok K. Mukherjee, April 2010 - July 2014.
- Junior Research Fellow, Department of Physics, Jadavpur University, under Prof. Alok K. Mukherjee, April 2008 - April 2010.
- Junior Research Fellow, Energy Research Unit, Indian Association for the Cultivation of Science under Prof. Debajyoti Das, July 2007 - April 2008.
- Junior Research Fellow, Department of Physics, Jadavpur University under Prof. Dipak Ghosh, July 2006 - July 2007.

University of Calcutta

- M.Sc, Physics, Electronics specialization, University of Calcutta, 2006
- B.Sc, Physics (Honours), S.A.Jaipuria College, University of Calcutta, 2003

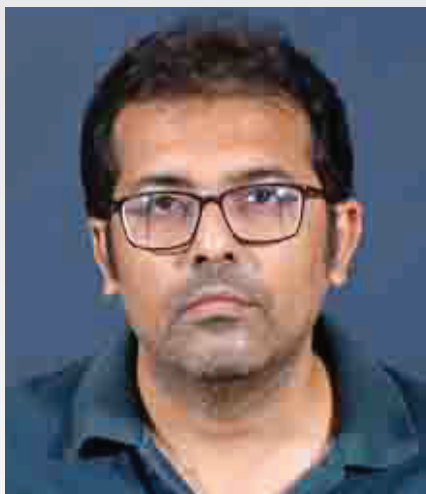
B.K.Paul's Institution

- Higher Secondary, West Bengal Council of Higher Secondary Education, B.K.Paul's Institution, 2000.
- Secondary, West Bengal Board of Secondary Education, B.K.Paul's Institution, 1998.

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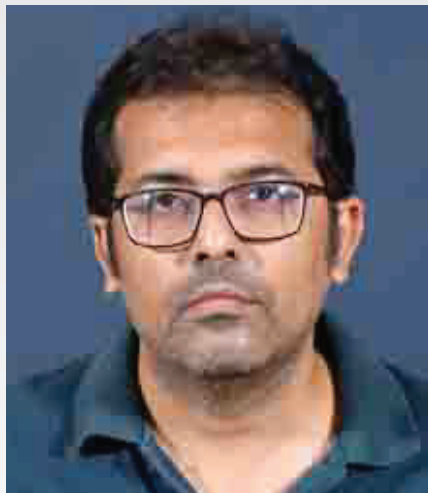
Academic Distinctions

- Qualified CSIR-UGC NET as a UGC JRF (Junior Research Fellowship) and LS (Eligible for Lectur - ership) in June, 2007.
- Qualified GATE 2007
- Qualified JEST 2006
- Qualified JEST 2005 (All India Rank 48)
- Nominated for National Scholarship in Higher Secondary Examination.
- Nominated for National Scholarship in Secondary Examination.

Teaching Experience

- Assistant Professor (Physics), Department of Physics, The Bhawanipur Education Society College, July. 2018 - Present
- Assistant Professor and Head of the Department (Physics), Department of Physics, Amity School of Applied Sciences, Amity University Kolkata, Sept. 2015 - July 2018
- Assistant Professor (Physics), Department of Basic Sciences, Batanagar Institute of Engineering, Science and Management, Sept. 2012 - Aug. 2015.
- Assistant Professor (Physics), Department of Applied Sciences, Haldia Institute of Technology, July 2011 - Sept. 2012.
- Part-Time Lecturer (Physics), Vijoygarh Jyotish Roy College, University of Calcutta, Nov. 2006 - July 2007.
- Part-Time Lecturer (Physics), Food and Nutrition Department, Calcutta Women's College, Universi - ty of Calcutta, Jan. 2007 - July 2007.





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Research Overview

My Ph.D. thesis titled "Crystal and molecular structure determination of some organic compounds and metal organic complexes using single -and powder-crystal X-ray diffraction" comprises of three parts, - (I) single crystal structural analyses of molecular materials, (II) Ab-initio structure determination of organic compounds as well as metal- organic complexes from laboratory X-ray powder diffraction data and (III) microstructural characterization of human kidney and pancreas stones using laboratory X-ray powder diffraction data.

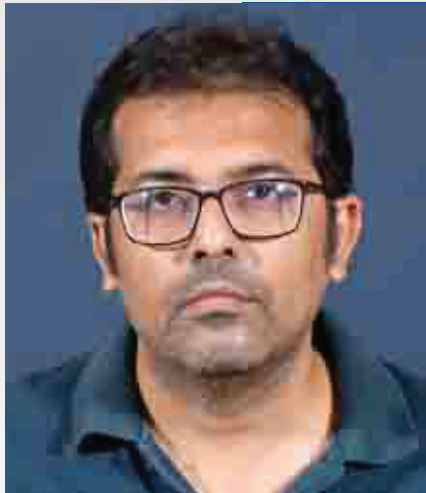
In single crystal X-ray analyses, I have used direct and Patterson methods for solving crystal structures and successfully tackled problem like disorder. When suitable single crystals are not available, I have explored the possibility of crystal structures solution from laboratory X-ray powder data. Although structure determination from X-ray powder data is not a straight forward job due to inherent limitations in the methodology, I have been successful in solving crystal structures of some organic and metal-organic compounds including one co-crystal using the recently developed direct space approaches followed by Rietveld refinement.

In order to interpret my crystallographic results, I've performed database analysis (using Cambridge Structural Database and programs included therein) and Hirshfeld surface analysis (using the program Crystal Explorer). I've also carried out theoretical calculations based on Density Functional Theory (DFT) to compare the crystallographic results with the optimized geometry and also to determine the electronic structures of the concerned compounds.

Additionally, I have performed quantitative phase analysis of some human kidney and pancreas stones from laboratory X-ray powder diffraction data using the Rietveld refinement method.

Currently I'm working on the hydrogen bonding nature and crystallographic arrangement of some Schiff base materials using Hirshfeld Surface and Fingerprint plot analysis and have a future plan to study the protein-ligand docking studies with those materials.





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Research Interest

- Hirshfeld Surface
- DFT
- Protein Ligand Docking
- Molecular Dynamics Simulation
- Drug Design

Administrative Assignment

Working as Nodal officer of West Bengal Student Credit Card Scheme from The Bhawanipur Education Society College, University of Calcutta.

Subjects Taught

Classical Mechanics | Physical Optics | Quantum Mechanics | Electrostatics | Statistical Mechanics | Solid State Physics | Nanotechnology

Major and Summer Projects

- In-silico screening of potential Active Pharmaceutical Ingredients (API) using quantum mechanical calculations Student: Anupa Bhattacharya, Department of Chemistry, Amity University Kolkata Status: Completed Year: 2016-17
- Structure solution of an unknown powder material using direct space technique using X-ray powder diffraction data. Student: Subhosree Das, Department of Chemistry, Amity University Kolkata Status: Completed Year: 2020-21
- Hirshfeld surface and fingerprint plot analysis of non-covalent interaction and interaction energies in the Schiff bases Student: Megha Sen Choudhury, Department of Chemistry, Amity University Kolkata Status: Completed but some papers are being ready for publication Year: 2020-21
- Study on non-covalent interaction and supramolecular arrangement for Heteronanostructures using Hirshfeld surface and fingerprint plot Analysis Student: Priya Poddar, Department of Chemistry -





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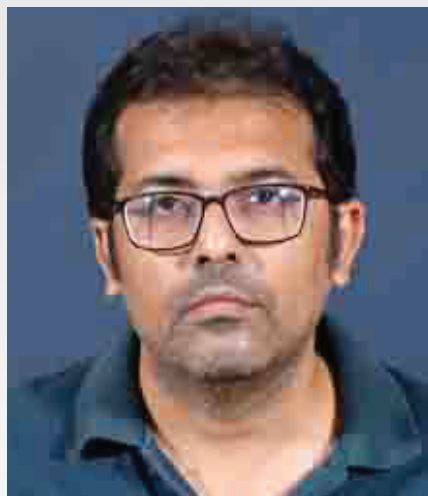
Faculty Development/ Orientation Program

Orientation Program organized by Teaching Learning Centre, Ramanujan College University of Delhi

Workshop/ Symposia

- Workshop on “Funding Opportunities and Success Stories of Capturing Research Grant”, Netaji Subhas Engineering College, Kolkata, India, July 2014 (Attended).
- 39 th National Seminar on Crystallography, University of Jammu, India, Oct. 2010 (2 Poster Presentations)
- 38 th National Seminar on Crystallography, University of Mysore, India, Feb. 2009 (Poster Presentation)
- Preparatory SERC School for Theoretical High Energy Physics, Indian Institute of Science, India, Oct. 2006 (Attended).
- C.K.Majumdar Memorial Workshop in Experimental Physics, S. N. Bose National Centre for Basic Sciences, Kolkata, India, July 2003 (Attended).
- “Nanomedicine: the future”, BES College, Sept. 2020 (Jt. convener)
- “The Enigma of Gravity: from apple to black hole”, BES College, July 2020 (Jt. convener)
- Neutrino: The Nobel connection” BES College, Aug. 2020 (Jt. convener)
- "Application of Quantum Mechanics in Nanomaterials", BES College, July 2021 (Jt. convener)





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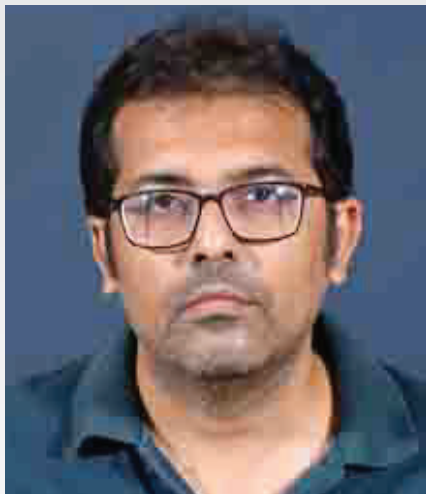
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Journal Publication

- A nimesulide derivative with potential anti-inflammatory activity: Synthesis, X-ray powder structure analysis and DFT study. Abir Bhattacharya, Kavitha Kankanala, Sarbani Pal and Alok K. Mukherjee. *Journal of Molecular Structure*, 2010, 975, 40–46.
- Crystal structure and electronic properties of two nimesulide derivatives: A combined X-ray powder diffraction and quantum mechanical study. Abir Bhattacharya, Soumen Ghosh, Kavitha Kankanala, Vangala Ranga Reddy, Khagga Mukkanti, Sarbani Pal and Alok K. Mukherjee. *Chemical Physics Letters*, 2010, 493, 151–157.
- Lamivudine hemihydrate. Abir Bhattacharya, Bhairab Nath Roy, Girij Pal Singh, Dhananjai Srivastava and Alok K. Mukherjee. *Acta Crystallographica Section C*, 2010, 66, o329–o333.
- A cyano-bridged bimetallic ferrimagnet: Synthesis, X-ray structure and magnetic study . Rupam Sen, Abir Bhattacharya, Dasarath Mal, Ashis Bhattacharjee, Philipp Gülich, Alok K. Mukherjee, Massimo Solzi, Chiara Pernechele and Subratanath Koner. *Polyhedron*, 2010, 29, 2762–2768.
- Tailor-made chiral pyranopyrans based on glucose and galactose and studies on self- assembly of some crystals and low molecular weight organogel (LMOG). Soumik Roy, Arijit Chakraborty, Basab Chattopadhyay, Abir Bhattacharya, Alok K. Mukherjee and Rina Ghosh. *Tetrahedron*, 2010, 66, 8512-8521.
- Naproxen and ibuprofen based acyl hydrazone derivatives: Synthesis, structure analysis and cytotoxicity studies. Mamatha Nakka, Murtuja Seikh Begum, B. F. Mathews Varaprasad, Lingam Venkata Reddy, Abir Bhattacharya, Madeleine Helliwell, Alok Kumar Mukherjee, Syed Sultan Beevi, Lakshmi Narasu Mangamoori, Khagga Mukkanti and Sarbani Pal. *Journal of Chemical and Pharmaceutical Research*, 2010, 2, 393-409.
- Tris(hydroxymethyl) aminomethane salt of ramipril: synthesis, structural characterization from X-ray powder diffraction and stability studies. Abir Bhattacharya, Basab Chattopadhyay, Santu Chakraborty, Bhairab N. Roy, Girij P. Singh, Himangshu M. Godbole, Umesh B. Rananaware and Alok K. Mukherjee. *Journal of Pharmaceutical and Biomedical Analysis*, 2012, 70, 280–287.





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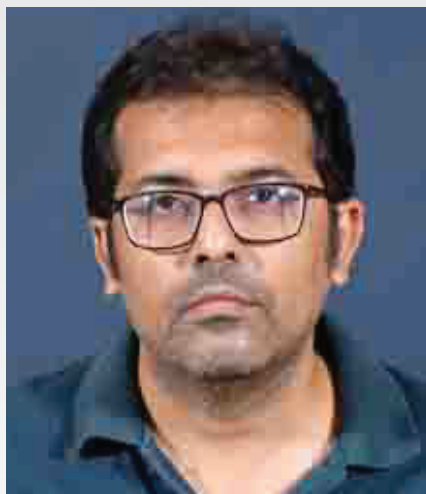
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Journal Publication

- Structural and microstructural characterization of seven human kidney stones using FTIR spectroscopy, SEM, thermal study and X-ray Rietveld analysis. Soumen Ghosh, Abir Bhattacharya, Paramita Chatterjee and Alok K. Mukherjee. *Zeitschrift für Kristallographie*, 2014, 229, 451–458.
- Three Nimesulide Derivatives: Synthesis, Ab Initio Structure Determination from Powder X-ray Diffraction, and Quantitative Analysis of Molecular Surface Electrostatic Potential Tanusri Dey, Paramita Chatterjee, Abir Bhattacharya, Sarbani Pal and Alok K. Mukherjee. *Crystal Growth & Design*, 2016, 8(12), 4517-4525
- Facile synthesis of doped ceria-based oxide by co-precipitation technique and performance evaluation in solid oxide fuel cell Shoroshi Dey, Debasmita Choudhury, Mayuri Choudhuri, Abir Bhattacharya, Jayanta Mukhopadhyay, Abhijit Das Sharma, Madhumita Mukhopadhyay *International Journal of Applied Ceramic Technology*, 2020, 17, 1769-1784
- Hirshfeld Surface Analysis as a “Novel Tool” for Studying Intermolecular Interactions in Cu Catecholase Complexes: A Guiding Tool for Future Application (s) *International Conference On Science, Engineering & Technological Innovation*, 2020, 35-38
- Probing the binding interaction of zinc (II) Schiff bases with bovine serum albumin: A spectroscopic and molecular docking study Megha Sen Chowdhury, Anwita Sarkar, Sristi Raj Rai, Sanchari Dasgupta, Ishani Majumder, Abir Bhattacharya, Debasis Das, Debosreeta Bose, Jayanta Mukhopadhyay, Madhumita Mukhopadhyay *Applied Organometallic Chemistry*, 2021, e6164
- Deciphering the Interaction of a Macrocyclic Tetranuclear Zn(II) complex with Biomimicking Surfactant: A Case Study using Cetyltrimethylammonium Bromide Anwita Sarkar, Sristi Raj Rai, Megha Sen Chowdhury, Tonmoy Mondal, Sanchari Dasgupta, Debasis Das, Abir Bhattacharya, Madhumita Mukhopadhyay and Debosreeta Bose *Biointerface Research in Applied Chemistry*, 2021, 11, in press
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Book Chapter

- Ab-initio Structure Determination of a Bimetallic Metal-organic Compound using Laboratory Powder X-ray Diffraction Data

- Abir Bhattacharya

THE IMPORTANCE OF INTERMOLECULAR INTERACTIONS IN SOLID-STATE X-RAYCRYSTAL STRUCTURES

Year 2016

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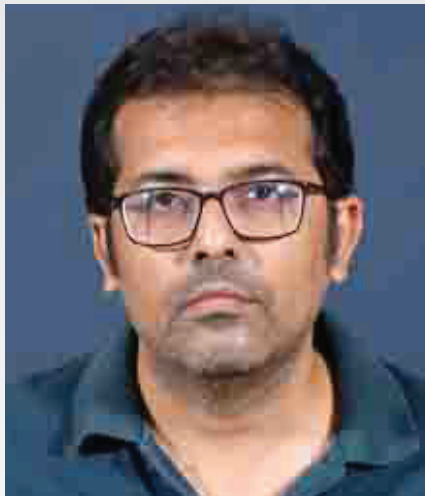
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Faculty Member

Date: 01st September, 2022



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Webinar

5/6/2020	Environmental development Committee BES College	Environment and climate change Concerns on WORLD ENVIRONMENT DAY
13/6/2020	Dept of Computer Science, BES College	Simplifying Artificial Intelligence, Machine Learning and Data Science
15/6/2020	Dept of Mathematics, BES College	History of Science, Science in History
20/6/2020	Dept of Mathematics, BES College	Application of Number Theory in Cyber Security: Few illustrations through Sage Math
22/6/2020	Dept of Physics, BES College	Saha and His Journey to the Stars
23/6/2020	Dept of Mathematics, BES College	The Sky And Beyond
25/6/2020	Dept of Chemistry, BES College	Pedagogical and Psychosocial Challenges.... Student's vision
26/6/2020	Dept of Chemistry, BES College	Pedagogical and Psychosocial Challenges.... Expert vision
27/6/2020	Dept of Electronics, BES College	One Dimensional Materials For Optoelectronic Devices
27/6/2020	Dept of Physics, Comp Science. Netaji Nagar College	Science and Technology for Sustainable Economic Growth in This Pandemic Scenario
8/7/2020	Dept of Physics, Surendra Nath College	A New View of the Solar System
11/7/2020	Teacher's Council and IQAC Netaji Nagar College for Women	Holistic Roadmap for Academic Excellence

