Dr. Dipak Kumar Sahoo

Post-Doctoral Fellow

Prof. Anindya Datta,

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Personal Information

Gender	Male
Marital Status	Married
Nationality	Indian
Date of Birth	12.02.1987
Permanent Address	S/O-Duryadhan Sahoo, Vil- Banamalipur Near Gadibrahma Primary school, Po-Banamalipur, Dist-Khurda, Odisha, India-752103.

Education and Research

Postdoc in chemistry	PI- Prof. Anindya Dutta	Dec 2020-now
PhD in chemistry	Under the supervision of Prof. Himansu S. Biswal, NISER-Bhubaneswar, Odisha, India	2014 - 2020
Master of Science (chemistry)	Pune University, Pune, India	2012-2014
Deputy Executive (Refrigeration)	Employee of a chemical and power based MNC Thermax Ltd, Pune, India	July 2009-Dec 2011
Bachelor of science	B.J.B. Autonomous College, Odisha, India	2006-2009

Research Experience

- Investigation of the solvation, dynamics and interactions of biomolecules in ionic liquids for their applications in biomedical and pharmaceutical areas using spectroscopic techniques.
- Synthesis of biocompatible, non-toxic and pharmaceutical active ionic liquids
- Biomolecules (protein, nucleobase and DNA) interactions, dissolutions, stability and activity study using spectroscopic techniques (UV-Vis, CD, FTIR, Raman, NMR (1D and 2D), fluorescence), microscopic techniques (FLIM, SEM,TEM) as well as computational techniques (Quantum chemical calculations, Molecular docking and MD simulations) which we use for our research work.
- The thermodynamic interpretation of biomolecules such as binding free energy, entropy changes and binding constants using isothermal titration calorimetry (ITC).
- I have previous experience of working about 2.5 years in Thermax Ltd after my B.sc chemistry where I was a deputy executive in refrigerator systems.

Technical Expertise

- Extensively used **UV-visible and Circular dichorism** spectroscopy to look at the structuaral, conformational and thermal stability of DNA and proteins (changes in **polypeptide backbone structure**) in ionic liquid (IL) and buffer solutions.
- Characterizing secondary structures of proteins (**amide I band analysis i.e. C=O stretching** vibration of peptide bond in 1700-1600 cm^{-1} region caused by change in backbone conformation and the hydrogen bonding pattern) by **FTIR spectroscopy** in presence of ionic liquids.
- **Raman spectroscopy** to characterize protein secondary structure looking at the change in position of **Amide I and III band of protein** on binding of ILs
- Used **NMR (1D, 2D) spectroscopy** to reveal dissolution mechanism of nucleobases in ionic liquids by observing chemical shift changes due to **C-H···O=C and N-H···O=C** hydrogen bond interactions. Also hand on experience of **solid state NMR** spectra recording and Powder XRD for solid samples..
- Working experience in using **steady state and time-resolved fluorescenc spectroscopy** for observing c**hanges in Trp microenvironment due to changes in protein conformation or binding of IL,** and also between **DNA and IL** binding sites in solvent environment.
- Hand on experience of using Fluorescence correlaton spectroscopy (**FCS**) and fluorescence lifetime imaging microscopy (**FLIM**) for studying proteins at single molecule level, and also **Femto second fluorescence up-conversion** laser spectroscopy.

- Experience in operating and analysing the data in Isothermal titration calorimetry (**ITC**), Differential scanning calorimetry (**DSC**) and Thermo Gavimetric Analysis (**TGA**) for determining thermodynamic properties (**binding free energy, binding enthalpy, entropy change, binding stoichiometry and binding constant**) of bimolecule-ionic liquids interactions.
- Experience in Field emission scanning electron microscope (**FE-SEM**), Transmission electron microscope (**TEM**), Dynamic light scattering (**DLS**) to observe **micro to nano meter scale size clusters, change in hydrodynamic radii, aggregation behavior and distribution of DNA, nucleobases and proteins in ionic liquid** solvent environment as a result of their interactions
- Trained in time of flight mass spectrometry (**TOF ESI-MS**), **GCMS, HPLC** techniques to characterize the synthesized ionic liquids and nucleobases
- Trained in using quantum chemical calculation program packages like **GAUSSIAN 09 and 16**, **GAMESS-USA**, and **TurboMole,** Natural Bond Orbital Analysis **(NBO 3.0, 6.0)**, Atom in Molecules Studies (**AIM-2000**), **Origin 8.0**, and visualization softwares like **VMD, Pymol, Gauss View, Argus Lab, Chem craft, and Chem Draw**.
- Also learned basics of MD Simulation (Used Gromacs software) and Molecular Docking
- Expert in writing manuscript for international journals, data analysis and proposal for research projects.

Teaching Experience

- Teaching Assistant in Physical chemistry courses and Laboratory such as Molecular Spectroscopy, Chemical Binding as part of my Ph. D program, NISER Bhubaneswar, 2014-2020
- Teaching Assistant in Physical chemistry courses and Laboratory such as Molecular Spectroscopy, Quantum Chemistry, IIT Bombay, 2020-current

Fellowships/Awards Availed

- Senior Research Fellowship- Department of Atomic Energy (DAE), Mumbai, Government of India (2016-present). NISER, Bhubaneswar, India
- Junior Research Fellowship - Department of Atomic Energy (DAE), Mumbai, Government of India (2014-2016), NISER, Bhubaneswar, India
- Qualified UGC-CSIR NET (National Eligibity Test)
- Best student in physical chemistry awarded – University of pune, India

Publications

☯ ***Publications in peer reviewed journals***

1. Shubhranshu Shekhar Choudhury, Subhrakant Jena, **Dipak Kumar Sahoo**, Shamasoddin Shekh, Rajiv K. Kar, Ambuj Dhakad, Konkallu Hanumae Gowd, and Himansu S. Biswal*, "*Gram-Scale Synthesis of 1,8-Naphthyridines in Water: The Friedlander Reaction Revisited*." (Accepted in **ACS Omega 2021**, DOI: 10.1021/acsomega.1c02798) (link)
2. Ambuj Dhakad, Subhrakant Jena, **Dipak Kumar Sahoo** and Himansu S. Biswal*, "*Quantification of the electric field inside protein active sites and fullerenes*." (Accepted in **PCCP 2021**, DOI: 10.1039/d1cp01769a) (link)
3. **Dipak Kumar Sahoo**, Kiran Devi Tulsiyan, Subhrakant Jena and Himansu S. Biswal*, "*Implication of Threonine-based Ionic Liquids towards the Structural Stability, Binding and Activity of Cytochrome c*." (**chemphyschem 2020**, 21, 1-12) (link)
4. **Dipak Kumar Sahoo**, Apramita Chand, Subhrakant Jena, Kiran Devi Tulsiyan, and Himansu S. Biswal*, "*Hydrogen-bond-driven Thiouracil Dissolution in Aqueous Ionic Liquid: A Combined Microscopic, Spectroscopic and Molecular Dynamics Study."* (**J. mol. Liq. 2020**, 319, 114275) (link)
5. Apramita Chand, **Dipak Kumar Sahoo**, Abhijit Rana, Subhrakant Jena, Himansu S. Biswal*, "The Prodigious Hydrogen Bonds with Sulfur and Selenium in Molecular Assemblies, Structural Biology and Functional Materials" (**Acc. Chem. Res. 2020,** 53, 8, 1580–1592) (link)
6. Juhi Dutta, **Dipak Kumar Sahoo**, Subhrakant Jena, Kiran Devi Tulsiyan, Himansu S. Biswal*, "*Noncovalent Interaction with Inverted Carbon: A Carbo-Hydrogen Bond or a New Type of Hydrogen Bond?"*(**Phys. Chem. Chem. Phys. 2020**, just accepted manuscript, https://doi.org/10.1039/D0CP00330A) (Link)
7. **Dipak Kumar Sahoo**, Subhrakant Jena, Kiran Devi Tulsiyan, Juhi Dutta, Suman Chakrabarty*, and Himansu S. Biswal*, "***Amino-Acid-Based Ionic Liquids for the Improvement in Stability and Activity of Cytochrome c: A Combined Experimental and Molecular Dynamics Study***." (**J. Phys. Chem. B 2019**, 123, 10100−10109) (Link)
8. **Dipak Kumar Sahoo**, Subhrakant Jena, Juhi Dutta, Abhijit Rana, Himansu S. Biswal*, "*Nature and Strength of M−H···S and M−H···Se (M = Mn, Fe, & Co) Hydrogen Bond*." (**J. Phys. Chem. A 2019**, 123, 2227−2236 **Published as part of The Journal of Physical Chemistry virtual special issue "Young Scientists"**) (Link)

9. Saurabh Mishra, **Dipak Kumar Sahoo**, Po-Jen Hsu*, Yoshiyuki Matsuda*, Jer-Lai Kuo*, Himansu S. Biswal*, and G. Naresh Patwari*, "*A liquid crucible model for aggregation of phenylacetylene in the gas phase."*(**Phys. Chem. Chem. Phys**., **2019**, 21, 13623—13632) (Link)

10. **Dipak Kumar Sahoo**, Subhrakant Jena, Juhi Dutta, Suman Chakrabarty,* Himansu S. Biswal*, "*Critical Assessment of the Interaction between DNA and Choline Amino Acid Ionic Liquids: Evidences of Multimodal Binding and Stability Enhancement*." (**ACS Cent. Sci. 2018**, 4, 1642−1651) (Link)

11. V. Rao Mundlapati, **Dipak Kumar Sahoo**, Suman Bhaumik, Subhrakant Jena, Amol Chandrakar, Himansu S. Biswal*, "*Noncovalent Carbon-Bonding Interactions in Proteins*." (**Angew. Chem. Int. Ed. 2018**, 57, 1 – 6) (Link)

12. V. Rao Mundlapati, **Dipak Kumar Sahoo**, Sanat Ghosh, Umesh Kumar Purame, Shubhant Pandey, Rudresh Acharya, Nitish Pal, Prince Tiwari, Himansu S. Biswal*, "*Spectroscopic Evidences for Strong Hydrogen Bonds with Selenomethionine in Proteins*." (**J. Phys. Chem. Lett. 2017**, 8, 794−800) (Link)

13. Sajal Kumar Patra, Kasturi Sahu, Bratati Patra, **Dipak Kumar Sahoo**, Sruti Mondal, Payel Mukherjee, Himansu S. Biswal*, Sanjib Kar*, "*Synthesis of urea derivatives via reductive carbon dioxide fixation into contracted porphyrin analogues***."** (**Green Chem., 2017**, 19, 5772–5776) (Link)

14. V. Rao Mundlapati, Sanjeev Gautam, **Dipak Kumar Sahoo**, Arindam Ghosh, Himansu S. Biswal*, "*Thioamide, a Hydrogen Bond Acceptor in Proteins and Nucleic Acids*." (**J. Phys. Chem. Lett. 2017**, 8, 4573−4579) (Link)

15. Ankit Singh[#], **Dipak Kumar Sahoo**[#], Srikant Kumar Sethi, Subhrakant Jena, Himansu S. Biswal*, "*Nature and Strength of the Inner-Core H···H Interactions in Porphyrinoids*." (**ChemPhysChem 2017**, 18, 3625 – 3633) (Link)

    # equal contribution

16. **Dipak Kumar Sahoo**; V. Rao Mundlapati; Arun A. Gagrai; Himansu S. Biswal* "*Efficient SO_2 Capture through Multiple Chalcogen Bonds, Sulfur-Centered Hydrogen Bonds and S•••π Interactions: A Computational Study*." (**ChemistrySelect 2016**, *1* (8), 1688-1694) (Link)

17. Arun A. Gagrai, V. Rao Mundlapati, **Dipak Kumar Sahoo**, H. Satapathy*, Himansu S. Biswal*, "*The Role of Molecular Polarizability in Designing Organic Piezoelectric Materials*." (**ChemistrySelect 2016**, *1* (14), 4326-4331) (Link)

Conferences

Poster Presentation

1. **XXVII IUPAP Conference on Computational Physics (CCP)**, organized by **IIT Guwahati and IMS Chennai** (2-5 DEC 2015). Title: "Green Ionic Liquids for Toxic SO_2 Capture: in silico screening of Cholinium-based Ionic Liquids with Pharmaceutically Active Anions"; Authors: **Dipak Kumar Sahoo** and Himansu S. Biswal.*
2. **30th Annual Conference of Orissa Chemical Society**, organized by **KIIT University, Bhubaneswar** (24-25 DEC 2016); Title: "Sulfur Centered Hydrogen Bond (SCHB): Its Strength and Application"; Authors: V. Rao Mundlapati, **Dipak Kumar Sahoo**, Subhrakant Jena and Himansu S. Biswal.*
3. **Spectroscopy and Dynamics of Molecules and Clusters (SDMC),** organized by **IISc, Bangalore at Pondicherry** (16-19 FEB 2017); "Efficient SO_2 Capture through Multiple Chalcogen Bonds, Sulfur-Centered Hydrogen Bonds and S···π Interactions: A Computational Study"; Authors: **Dipak Kumar Sahoo,** V. Rao Mundlapati, Arun Anand Gagrai, and Himansu S. Biswal.*
4. **INTER IISER & NISER CHEMISTRY MEET**, Organized by NISER, Bhubaneswar (22-24 DEC 2017); Title: "Nature and Strength of the Inner Core H···H Interactions in Porphynoids"; Authors: **Dipak Kumar Sahoo,** Ankit Singh, Srikant Kumar Sethi, Subhrakant Jena and Himansu S. Biswal*
5. **Spectroscopy and Dynamics of Molecules and Clusters (SDMC),** organized by **IISER Kolkata, IACS Kolkata, SINP Kolkata at SINCLAIRS RETREAT, DOOARS (near Darjeeling)** (15-18 FEB 2018); Title: "Anti-electrostatic Hydrogen Bonds with Transition Metal Hydrides: A Deviation from IUPAC definition of Hydrogen bonds"; Authors: **Dipak Kumar Sahoo,** Himansu S. Biswal*
6. **Spectroscopy and Dynamics of Molecules and Clusters (SDMC),** organized by **IISER Mohali, IIT Kanpur at Koti resorts, Shimla** (21-24 FEB 2019); Title: "Understanding DNA-IL binding for long term storage and application through comprehensive experiment and computational studies"; Authors: **Dipak Kumar Sahoo,** Himansu S. Biswal*
7. **Fluorescence Correlation Spectroscopy (FCS),** organized by **TIFR Hyderabad, Hyderabad** (16-21 DEC 2019); Title: "Stability and Activity study of Cytochrome-c in Ionic Liquid using various Spectroscopic and computational methods"; Authors: **Dipak Kumar Sahoo,** Himansu S. Biswal*

Oral Presentation

- **NATIONAL BIOORGANIC CHEMISTRY CONFERENCE (NBCC)**, Organized by NISER, Bhubaneswar (22-24 DEC 2018); Title: "Critical Assessment of the

Interaction between DNA and Choline Amino Acid Ionic Liquids (CAAILs): Evidences of Multi-Modal Binding and Stability Enhancement."

- **22nd REGIONAL CONFERENCE OF ORISSA CHEMICAL SOCIETY and STATE LRVEL SEMINAR ON "GREEN CHEMISTRY: SOLUTION TO ENVIRONMENTAL CRISIS"**, Organized by OCS, Kendrapara, Odisha (3rd NOV 2019); Title: "Cation and Anion Based Amino-Acid Ionic-Liquids: An Efficient Green Source for Structural Stability and Catalytic Activity of Cytochrome-c Protein."

Declaration

I declare that the information given above is true to the best of my knowledge and belief and nothing has been hidden.

Dr. Dipak Kumar Sahoo